

Model Evaluation Workgroup
Technical Memorandum 2f

Estimation of Sediment Bed Properties for Green Bay

Prepared by:
Wisconsin Department of Natural Resources

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1.0 SUMMARY

This technical memorandum is provided in partial fulfillment of the Memorandum of Agreement (“Agreement”) between the State of Wisconsin and seven paper companies (“Companies”), dated January 31, 1997.

Model evaluations will be undertaken according to the procedures discussed in the “Workplan to Evaluate the Fate and Transport Models for the Lower Fox River and Green Bay” (“Workplan”). This Workplan was developed by Limno-Tech, Inc. (LTI) on behalf of the Companies and the Wisconsin Department of Natural Resources (WDNR) and was conditionally approved by WDNR on September 26, 1997. This technical memorandum is an extension of the Task 2 series of model evaluation work products, and is entitled “Analysis of Sediment Bed Properties for Green Bay.”

Numerous investigations of Green Bay sediments provide information about sediment bed properties at discrete points in space (and time). However, no investigation can provide information about sediment properties through the entire spatial and volumetric extent of the sediment bed without additional analysis. The results of these studies must be interpolated in a consistent and technically sound manner to provide a continuous representation of sediment bed properties. The objective of this technical memorandum is to present a methodology to estimate sediment bed properties from the results of field investigations and its application to Green Bay, to estimate the physicochemical properties of the sediment bed. One specific intent of this work effort is to provide a single, consistent set of interpolated sediment bed properties for use in model evaluation and State of Wisconsin-led Natural Resources Damage Assessment (NRDA) and Superfund (CERCLA) Remedial Investigation/Feasibility Study (RI/FS) and Risk Assessment (RA) efforts.

The selected interpolation approach utilized the Grid module in ARC/INFO 7.1.2 geographic information system (GIS) and ArcView 3.1 with the Spatial Analyst 1.1 extension, raster data (grids), and the inverse distance weighting (IDW) technique. The selected grid cell size was 100 meters by 100 meters. The selected IDW weighting exponent was 2. The selected radius of influence was 8,000 meters.

Within Green Bay, “soft” sediments were inferred to exist over approximately 52% of the total surface area of the bay. Within the inferred soft sediment area, the estimate of the contaminated sediment volume was 622,353,000 m³. The estimate of the sediment polychlorinated biphenyl (PCB) mass inventory was 69,955 kg. Other sediment bed properties interpolated within Green Bay are depth of analysis (a surrogate for sediment thickness), dry bulk density, total organic carbon (TOC), particle size distribution, Cesium-137, and Lead-210.

These interpolations infer sediment bed properties for approximately 52% of the total surface area of the bay. Null (“no data”) values were assigned to the remaining surface area of the bay. Null values indicate that no sediment bed properties were inferred at a location because of either of two conditions: 1) contaminated sediments are not believed to exist at that horizontal or vertical

location; or 2) contaminated sediments may exist but the location was too distant from the nearest sample collection point for properties to be estimated. It should be noted that PCB contaminated sediments may exist in unsampled regions of Green Bay. For example, the area associated with the path of the Lower Fox River “plume” is largely unsampled. The estimates of contaminated sediment volume and PCB mass inventory may therefore represent lower bound estimates.

2.0 INTRODUCTION

2.1. PURPOSE OF THIS DOCUMENT

To complete the model evaluation process as described in the Agreement, the physicochemical properties of the Lower Fox River and Green Bay sediment beds must be estimated. These estimated properties are necessary to define model initial conditions as well as spatial conditions of the Lower Fox River/Green Bay system for the temporal (point-in-time) analysis of model performance. The purpose of this document is to present:

1. A methodology to estimate sediment bed properties; and
2. Application of this methodology to Green Bay and estimated sediment bed properties.

Sediment bed properties for the Lower Fox River are not estimated or presented in this document.

2.2. OVERVIEW

Several investigations of Green Bay sediments have been completed historically (see Figure 2-1 for study area map). Each of these investigations provides information about sediment bed properties at discrete points in space and time. However, no investigation can provide information about sediment properties through the entire sediment bed without additional analysis. Therefore, the results of each study must be interpolated in a consistent and technically sound manner to provide a continuous representation of sediment bed properties. The objective of this technical memorandum is to present a methodology to estimate sediment bed properties from the results of field investigations and its application to Green Bay to estimate the physicochemical properties of the sediment bed. One specific intent of completing this work effort is to provide a single, consistent set of interpolated sediment bed properties for use in model evaluation and State of Wisconsin-led Natural Resources Damage Assessment (NRDA) and Superfund (CERCLA) Remedial Investigation/Feasibility Study (RI/FS) and Risk Assessment (RA) efforts.

Selection of a sediment bed interpolation technique is discussed in Section 3.0. The selected interpolation technique is the basis for development of a sediment bed model for Green Bay. Sediment bed property definitions, data sources, data handling, and selection of site-specific parameter values for the sediment bed model are discussed in Section 4.0.

The results of the Green Bay sediment bed property estimations are presented in Section 5.0. The estimated sediment bed properties presented in this technical memorandum are:

1. Total polychlorinated biphenyls (PCBs, ug/kg)
2. Total organic carbon (TOC, %)

3. Dry bulk density (g/cm^3)
4. Depth of analysis (meters)
5. Cesium-137 (pC/g)
6. Lead-210 (pC/g)
7. Particle size (% sand/silt/clay)

Data were interpolated for five vertical sediment layers. The stratification used, in distance from the sediment-water interface, was:

Layer	Depth (cm)
1	0 – 2
2	2 – 4
3	4 – 6
4	6 – 10
5	> 10

Section 6.0 discusses uncertainties associated with spatial and temporal variation in data, and with the interpolation parameters that are used.

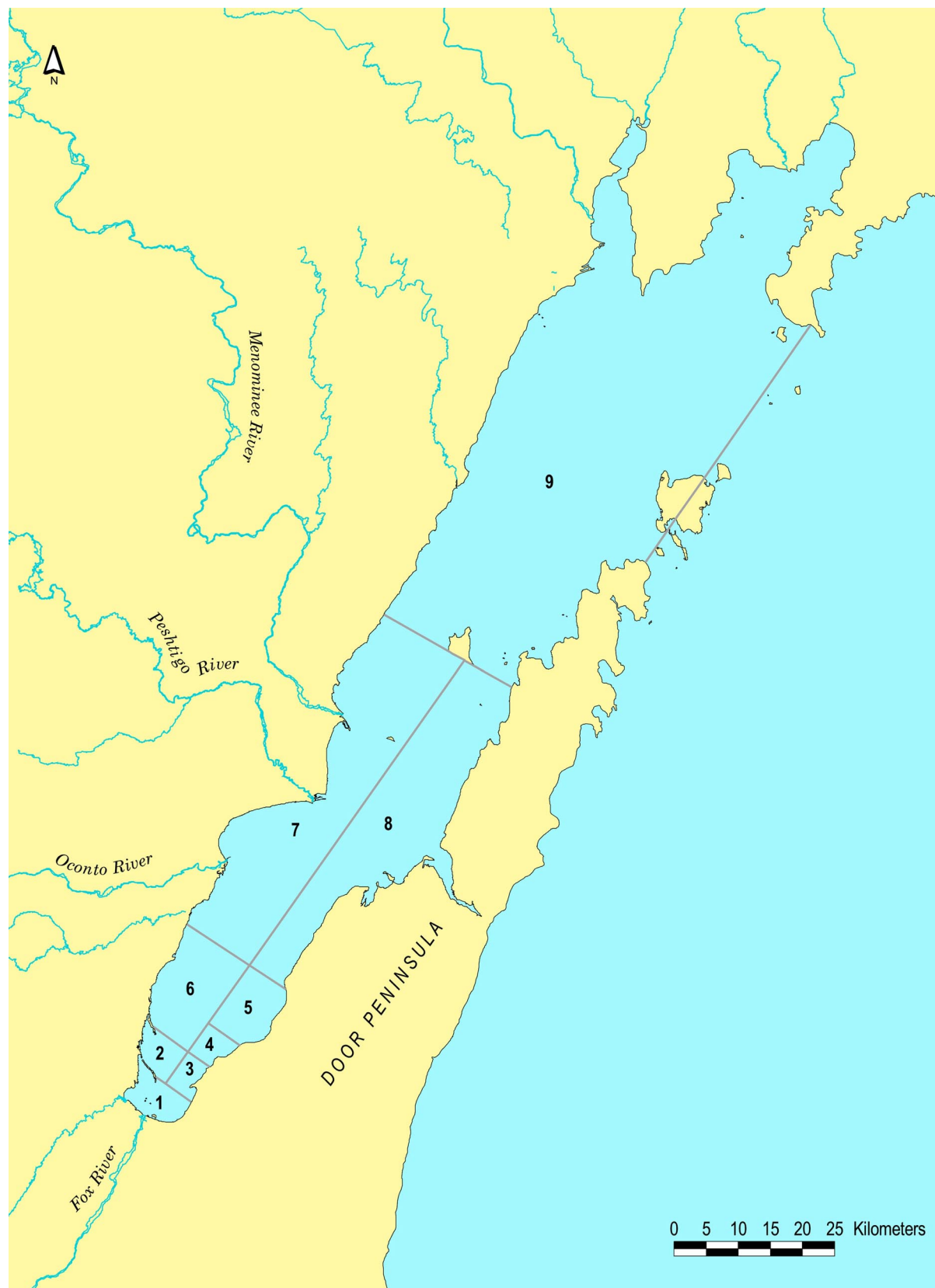


Figure 2-1. Green Bay study area with GBTOX model segmentation (segments labeled 1-9).

3.0 SELECTION OF SEDIMENT BED INTERPOLATION TECHNIQUE

In order to estimate the physicochemical properties of the Green Bay sediment bed, a geographic information system (GIS) was selected to interpolate from known locations of sampled sediments. A GIS provides the necessary tools for estimating both the spatial extents and values of bed properties. The GIS can be used to set boundary conditions based on location of bed and shoreline features. It is designed to store location information, as well as attribute information associated with locations. The GIS can also be used to visualize data distributions and interpolation results (WDNR 1999).

For Task 2e, GIS-based interpolation frameworks were tested and it was found that a raster-based (cell-based) framework is a better choice than other methods for sediment bed interpolation (WDNR 1999). That framework was applied for interpolation of Green Bay sediment bed properties. ARC/INFO Version 7.2.1 for Windows NT and ArcView 3.1 with the Spatial Analyst 1.1 extension were the selected GIS. Spatial data layers developed and used within ARC/INFO can be accessed readily by users of ArcView GIS. Use of the ARC/INFO Grid module for Green Bay sediment bed property interpolation is consistent with use of ArcView and Spatial Analyst for interpolation of Lower Fox River sediment properties as performed in Task 2e.

Inverse distance weighting (IDW) was selected as the interpolation technique that was applied in the GIS. In the IDW technique, known values at nearby locations affect each interpolated value more than known values farther away. IDW estimates values for unsampled locations as an average of sample values within its vicinity (Berry 1995). This average is weighted, so the influence of surrounding values decreases with distance from the location being estimated. IDW is represented by the expression:

$$C_{x,y} = \frac{\sum_{i=1}^m C_i d_i^{-n}}{\sum_{i=1}^m d_i^{-n}} \quad \text{for } m \text{ observations within distance } r$$

where: $C_{x,y}$ = interpolated value at location x,y

C_i = observed value at location i

d_i = distance between location i and x,y

n = exponent that weights the influence of observed value on $C_{x,y}$

m = number of observations within radius r of location x,y

r = radius of influence around location x,y

With IDW, observed values are preserved and the range of interpolated values is limited to the minimum and maximum of the original observed data (Watson and Philip, 1985; Hu, 1995).

For Task 2e, this technique was tested against other tools available in GIS and found to be superior for estimations of sediment bed properties in the Lower Fox River (WDNR 1999). The Task 2e evaluation criteria for interpolation testing were:

1. Interpolated values can never be less than zero.
2. The underlying mathematics of the interpolation technique should be readily understood and communicable to a wide audience.
3. The computational effort needed to complete a test interpolation should not exceed 10 hours of processing time (if possible).

IDW met those criteria. Spline methods were ruled out due to the potential for abrupt changes in estimated values over short distances and the potential for negative interpolated values. Kriging potentially yields negative estimated values, has mathematics that are not readily explained, and can have inordinate computing times. Technical Memorandum 2e provides a more detailed explanation of IDW and other interpolation methods.

4.0 SEDIMENT BED PROPERTY DATA

A model for interpolating Green Bay sediment bed properties was developed. A geographic information system with raster-based analysis tools was chosen to perform interpolations. ARC/INFO 7.2.1 and ArcView 3.1 with the Spatial Analyst 1.1 extension were used. The inverse distance weighting (IDW) method was selected as the interpolation technique. This section describes the sediment bed properties that were interpolated, the data used as inputs to the interpolation, and the selection of IDW parameters used in the GIS. Results of interpolations of Green Bay sediment bed properties are discussed in Section 5.0.

4.1. DEFINITION OF SEDIMENT BED PROPERTIES

The estimated sediment bed properties presented in this technical memorandum are:

1. Polychlorinated biphenyls (PCBs) (ug/kg)
2. Total organic carbon (TOC) (%)
3. Dry bulk density (g/cm³)
4. Depth of analysis (sediment thickness) (m)
5. Cesium-137 (pC/g)
6. Lead-210 (pC/g)
7. Particle size (% sand/silt/clay)

PCBs are defined as the total PCB concentration associated with particles on a dry weight basis. Where PCBs were quantified on an individual congener basis, the congener values were summed to represent the total PCB concentration. Where PCBs were quantified on an individual aroclor basis, the aroclor values were summed to represent the total PCB concentration. The method detection limit (MDL) for congener samples ranged from 0.001 ug/kg to 124 ug/kg. The MDL for aroclor 1242 in sediment samples collected by BBL (1999) ranged from 5.7 ug/kg to 81 ug/kg.

Total organic carbon (TOC) is defined as the organic carbon content of dry sediment particles. TOC is a “mixture of plant and animal products in various stages of decomposition; it consists of compounds synthesized biologically and chemically from degradation products, and of microorganisms and their decomposing remains” (Wetzel 1983). Sediment TOC is presented as a percentage of sediment mass.

Dry bulk density is the mass of dry sediment particles per unit volume at the in-situ porosity of the sediments. Dry bulk density is computed from water content (reported as % moisture or % solids) and particle density (specific gravity).

Depth of analysis is a surrogate for sediment thickness. Total sediment thickness data for Green Bay do not exist so a surrogate is necessary. Depth of analysis is defined as the maximum depth in the sediment column for which a sample was analyzed (i.e. the deepest recorded core slice at a sampling location for which a laboratory analysis). Depth of analysis represents a lower bound estimate of the total vertical extent of sediments.

Cesium-137 and Lead-210 are the concentration [activity] of a specific radioactive isotope of cesium and lead, respectively, measured in each sediment interval in pCi/g of sediment, on a dry weight basis. Cs-137 and Pb-210 were determined nondestructively on dried sediment samples by gamma-ray spectrometry (Manchester, 1993).

Particle size distribution refers the distribution of different sized particles within a sample. Sediment particle size distribution is reported as the percent of a sample that consists of sand, silt and clay sized particles.

4.2. GREEN BAY SEDIMENT BED PROPERTY DATA SOURCES

A literature search was performed to construct the most complete data set possible for sediment bed mapping efforts. This search included queries of: University of Wisconsin Sea Grant Institute, University of Wisconsin campuses in Milwaukee, Madison, and Green Bay, the Center for Great Lakes Research, Illinois State Geological Survey, USEPA Large Lakes Research Station (LLRS), USEPA Great Lakes National Program Office (GLNPO), NOAA Great Lakes Environmental Research Laboratory (GLERL), NOAA Great Lakes Data Rescue, the Integrated Paper Services laboratory, Wisconsin State Laboratory of Hygiene, U.S. Army Corps of Engineers, Green Bay Metropolitan Sewage District, United States Geological Survey, U.S. Fish and Wildlife Service, Wisconsin Department of Natural Resources, and the University of Michigan. Data sources are presented in Table 4-1.

Data obtained from this literature search encompassed the thirty-year period between 1968 and 1998. These data included over one hundred physical and chemical sediment parameters. For consistent treatment of data, horizontal and vertical location information is needed. Ideally, each sample should have a start and end depth to be included in an interpolation. Unfortunately, start and end depths were not reported for all samples. For example, surface sediment grab samples do not generally report end depths. While knowledge of sampling devices could be used to estimate the depth interval for which a sample applied, information describing sample collection devices or methods was not always reported. Since consistent treatment of data was not possible, data without sample start and end depths were excluded from subsequent interpolations.

In addition to the properties identified for interpolation in Section 4.1, data for several other parameters exist. These properties include phosphorus, total carbon, and chemical oxygen demand (COD) from which sediment oxygen demand (SOD) may be inferred. Unfortunately, these data are available for only a small portion of the surface area and depth of bay sediments. Due to their sparseness, no interpolations of these properties were performed.

Table 4-1. Data sources for estimation of Green Bay sediment bed properties.

Data Source	Year Collected	Bulk Density	Solids	Porosity	Particle Size	TOC	Total Carbon	PCB : Total Homolog	PCB: Congeners	PCB: Aroclors	Water Content	Phosphorous	Chemical Oxygen Demand (COD)	Cs-137	Pb-210
Ankley et al. (1992)	1988					X			X						
BBL (1999)	1998		X			X			X	X				X	X
Buelow (1982)	1980									X					
Cahill (1981)	1975				X	X									
Chen et al. (1983)	1972-74	X			X	X									
Eadie et al. (1991)	1989					X									
GBMBS: Andren Surveys, 1987-90	1987-90							X	X		X				
Manchester et al. (1996)															
GBMBS: Edgington Surveys, 1986-91	1986-91			X		X					X			X	X
Manchester et al. (1996)															
Hermanson et al. (1991)	1981, 1983									X					
IPS (1995)	1994				X										
Karls (1997)	1995						X							X	X
Miller (1986)	1985				X										

Table 4-1 (continued). Data sources for estimation of Green Bay sediment bed properties.

Data Source	Year Collected	Bulk Density	Solids	Porosity	Particle Size	TOC	Total Carbon	PCB : Total Homolog	PCB: Congener	PCB: Aroclors	Water Content	Phosphorous	Chemical Oxygen Demand (COD)	Cs-137	Pb-210
Moore et al. (1973)	1968-69				X										
Su (1997)	1995	X		X											
USACE (1995)	1994	X	X		X	X						X	X		
USACE (1995)	1995									X					
USACE (1999)	1998	X	X	X	X	X			X	X		X	X		
USEPA STORET Database-Michigan	1969, 1975, 1976		X	X		X				X		X	X		
USEPA STORET Database-Wisconsin	1968-1970, 1974, 1975, 1977, 1981, 1990, 1992		X	X		X	X	X		X		X	X		
WDNR (1998)	1995				X	X				X	X				

4.3. DATA HANDLING OPERATIONS

Prior to spatial analysis, it was necessary to standardize the sediment bed data. Consistency in measurement units is critical to successful interpolation. All data were reviewed to determine the original units of measure used for reporting. The data were then transformed to consistent units of measure. All sediment sample depth data were converted to consistent units of measure (meters). The datum for all sediment sample depths was the sediment-water interface. Sediment bed property measurements were also converted to consistent units. The units for each property were listed previously in Section 4.1.

Location data for sampling points were standardized by using a consistent projection and coordinate system. All coordinates were transformed to the Wisconsin Transverse Mercator (WTM) projection using the North American Datum of 1927 (NAD 27) reference datum. The WTM projection is the standard for WDNR surveying and GIS efforts. Use of the NAD 27 datum was consistent with the data handling operations performed as part of Task 2e (WDNR, 1999).

4.4. DATA SETS USED TO ESTIMATE SEDIMENT BED PROPERTIES

4.4.1. TOTAL PCBs

PCBs are defined as the total PCB concentration associated with particles on a dry weight basis. Total PCB concentrations were computed as the sum of congener or aroclor observations for each sample. For all congener and aroclor summations, values recorded as being below the method detection level (MDL) were treated as zero. This treatment represents an analytical lower bound and yields the lowest possible total PCB concentration for that sample.

PCB observations from the GBMBS, BBL (1999), and WDNR (1998) data sets were used for interpolations. Data from the remaining sources were not included as a consequence of missing or otherwise inadequate horizontal or vertical location information. Figure 4-1 shows the locations of the PCB data used in the interpolations.

To account for variation with depth in the sediment column, sediment PCB concentrations were interpolated for each of five depth intervals (layers) as follows:

1. 0 - 2 cm
2. 2 - 4 cm
3. 4 - 6 cm,
4. 6 - 10 cm; and
5. > 10 cm.

Prior to interpolation, a thickness-weighted PCB concentration was computed for each depth interval at each core location.

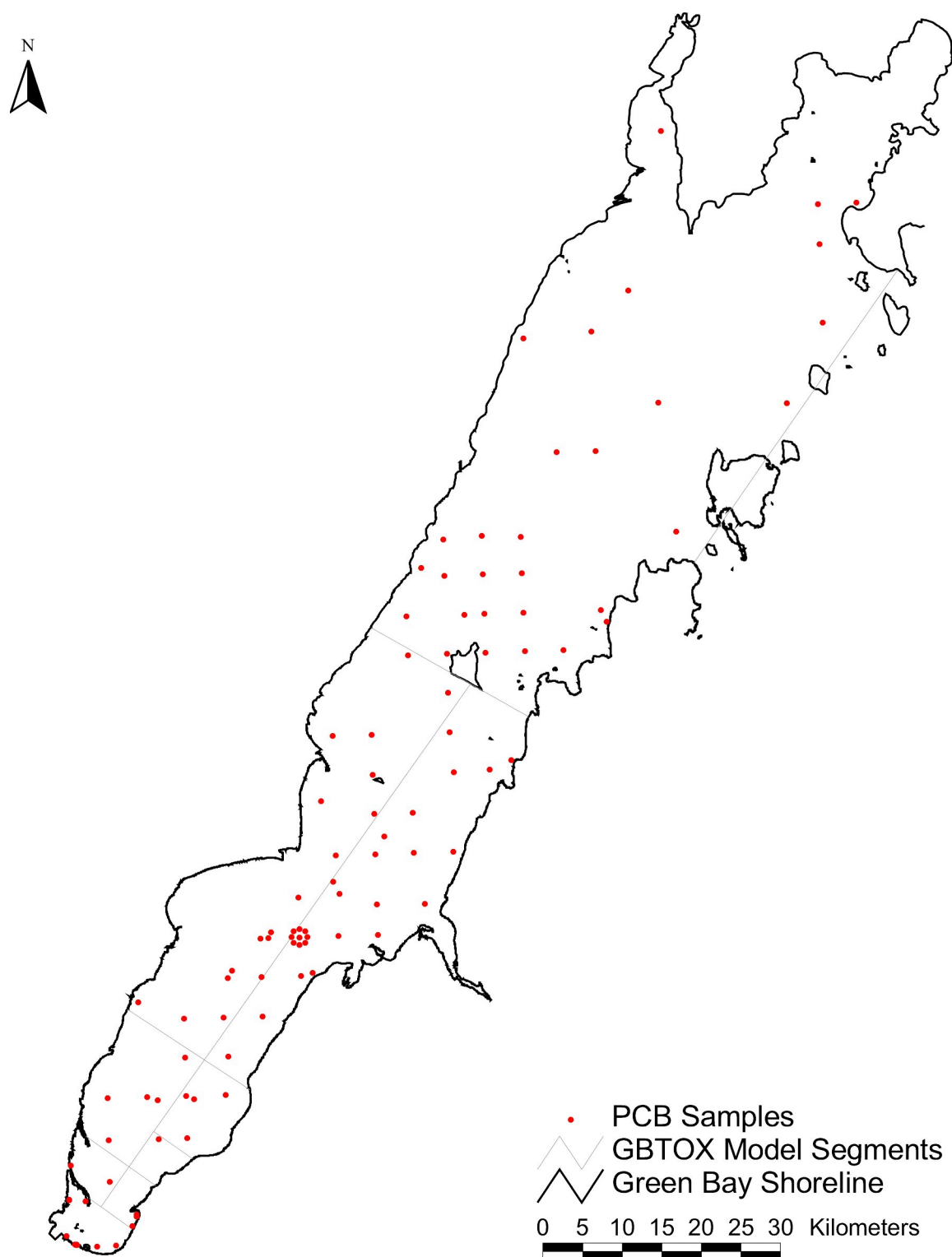


Figure 4-1. Total PCB sample locations.

4.4.2. TOTAL ORGANIC CARBON

Total organic carbon (TOC) is the organic carbon content of dry sediment particles. TOC is expressed as a percentage of the dry sediment weight. TOC observations from the GBMBS data set were used for interpolations. Data from the remaining sources were not included as a consequence of missing or otherwise inadequate horizontal or vertical location information. Prior to interpolation, a thickness-weighted TOC concentration was computed for each depth interval at each core location. Figure 4-2 shows the locations of the TOC data used in the interpolations.

4.4.3. DRY BULK DENSITY

Dry bulk density is the mass of dry sediment particles per unit volume at the in-situ porosity of the sediments (g/cm^3). Dry bulk density was estimated from porosity observations and particle density. An average particle density of $2.45 \text{ g}/\text{cm}^3$ as employed in Technical Memorandum 2e Lower Fox River sediment bed properties (WDNR 1999) was used in the dry bulk density analysis.

The formula used to calculate dry bulk density from porosity is:

$$P_b = P_p (1 - \phi)$$

where: P_b = dry bulk density (g/cm^3)

P_p = particle density (g/cm^3)

ϕ = porosity = pore volume / total volume

Bulk density observations (or estimates computed from porosity) from the GBMBS, BBL (1999), and WDNR (1998) data sets were used for interpolations. Data from the remaining sources were not included as a consequence of missing or otherwise inadequate horizontal location information. Prior to interpolation, a thickness-weighted bulk density was computed for each core location. Bulk density was then interpolated as a constant with depth at each location (i.e. interpolated values do not change with depth). Figure 4-3 shows the locations of the bulk density data used in the interpolations.

4.4.4. DEPTH OF ANALYSIS

Depth of analysis is defined as the maximum depth in the sediment column for which a sample was analyzed (i.e. the deepest recorded core slice obtained at a sampling location for which a laboratory analysis was performed). Depth of analysis is a surrogate for used to estimate sediment thickness since total sediment thickness for data Green Bay do not exist. Depth of analysis represents a lower bound estimate of the total vertical extent of sediments.

4.4.5. Cs-137 AND Pb-210

Cs-137 and Pb-210 are defined as the concentration [activity] of specific radioactive isotopes of cesium and lead, respectively, on a dry weight basis (pC/g). Cs-137 and Pb-210 observations from the GBMBS and the BBL (1999) data sets were used for interpolation. Of these data, the

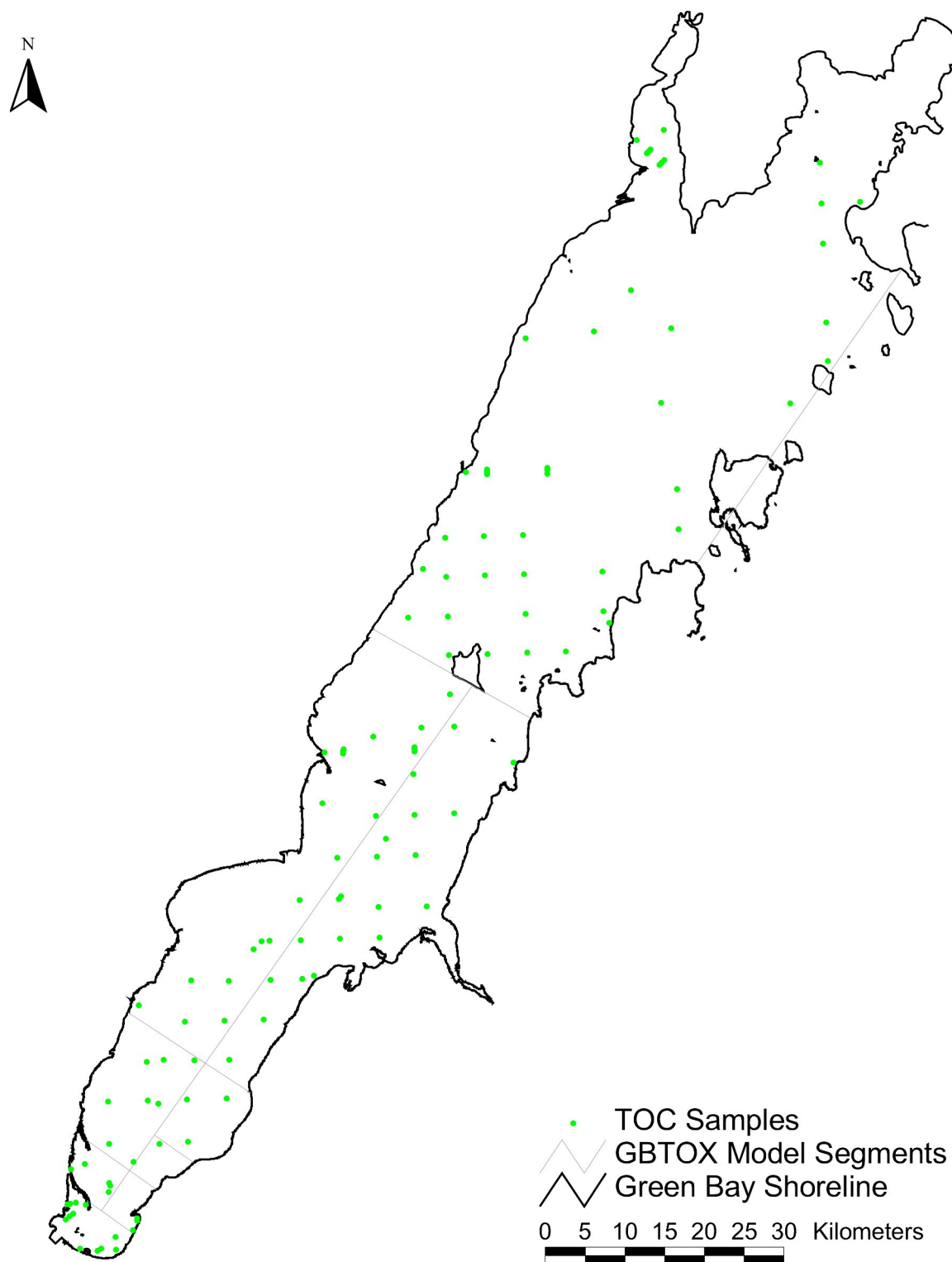


Figure 4-2. TOC sample locations.

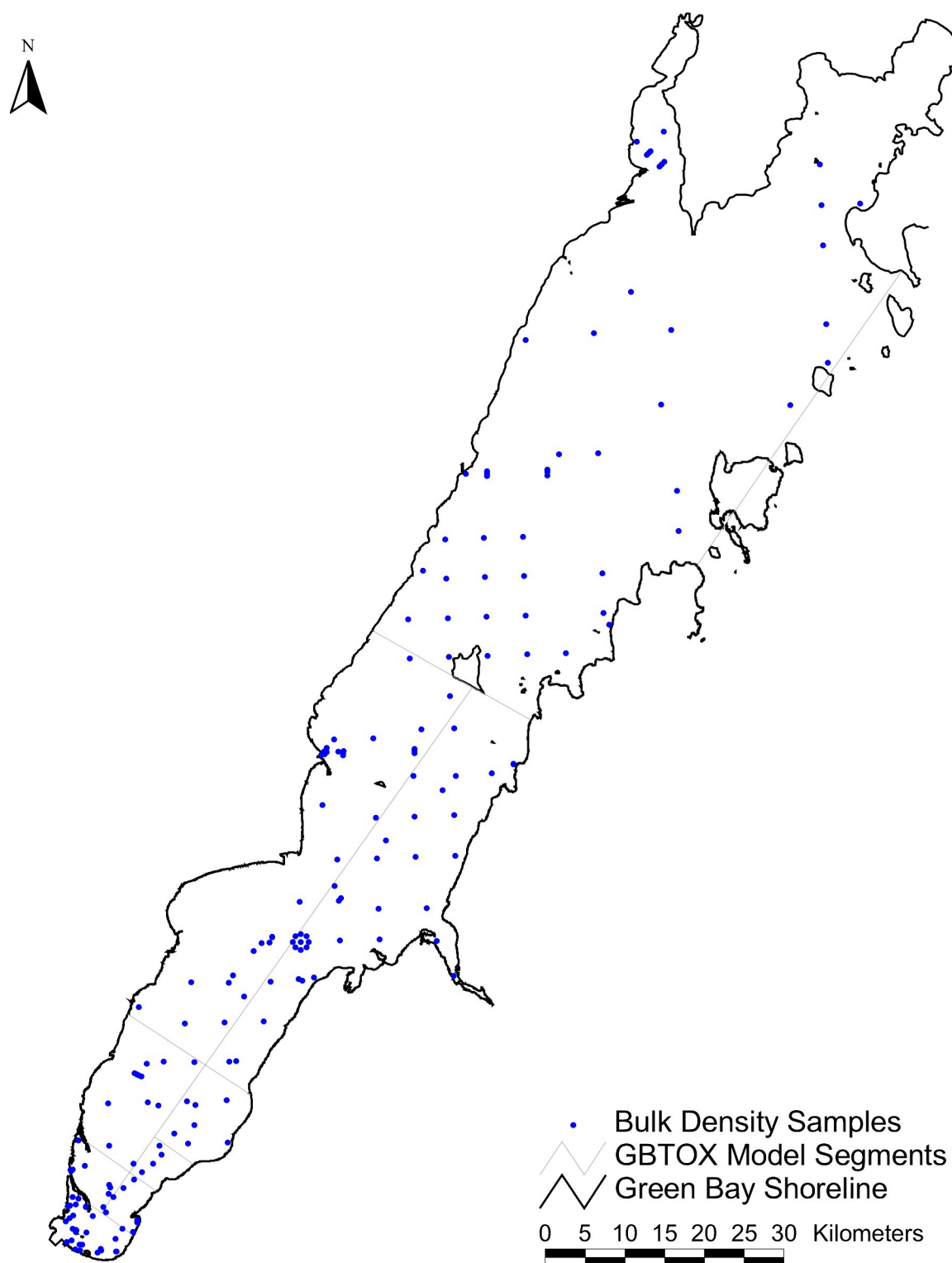


Figure 4-3. Bulk density sample locations.

samples from one core site were not included due to missing location information. Figures 4-4 and 4-5 show the location of Cs-137 and Pb-210 data used in the interpolations.

4.4.6. PARTICLE SIZE (% SAND/SILT/CLAY)

Particle size refers to the distribution of different sized particles within a sediment sample and presented as the percent of sand, silt, and clay sized particles. Particle size data were collected between 1972 and 1994, including 486 samples. Locational information was available for 35 locations. However, depth information was available for only 15 of these 35 sample locations. Reported particle size distributions are presented for Layers 1 in Figures 4-6 to 4-10. Figure 4-11 presents the locations of those samples for % sand, % silt, and % clay with no depth information.

4.5. SELECTION OF INTERPOLATION TECHNIQUE PARAMETER VALUES

Several parameters must be specified when using IDW interpolation within ARC/INFO or ArcView GIS. Each combination of parameters provides a different interpolation result. An optimal combination provides accurate predicted values, a wide coverage of the study area, appropriate spatial precision, and reasonable computing speeds. Specified parameters are discussed below and include:

- The weighting exponent n
- The method for isolating data points that influence any particular interpolated value
- The radius of influence r
- Designation of barriers to limit the extent of interpolations
- Grid cell size for analysis

4.5.1. IDW WEIGHTING EXPONENT

The weighting exponent n affects the influence that observed data points have on interpolated values. In general, the farther away a data point is from a cell, the less influence that point will have on the interpolated value in that cell. As the weighting exponent increases, the influence of distant data points decreases and the influence of nearby data points increases.

Selecting a reasonable value for n is not a trivial task. As the exponent is lowered, the closer each estimated value approximates the overall mean of the observed data points. As the exponent is increased, the closer the estimation approximates Thiessen polygons where each location is given the value of the single nearest observed data point (Hu, 1995; Watson and Philip, 1985). A reasonable exponent value provides a middle ground between these two extremes, allowing nearby points to have the most influence while still allowing some information to be provided by more distant points. Very distant points can be excluded from having any influence by the use of a limiting radius around estimated points (discussed below).

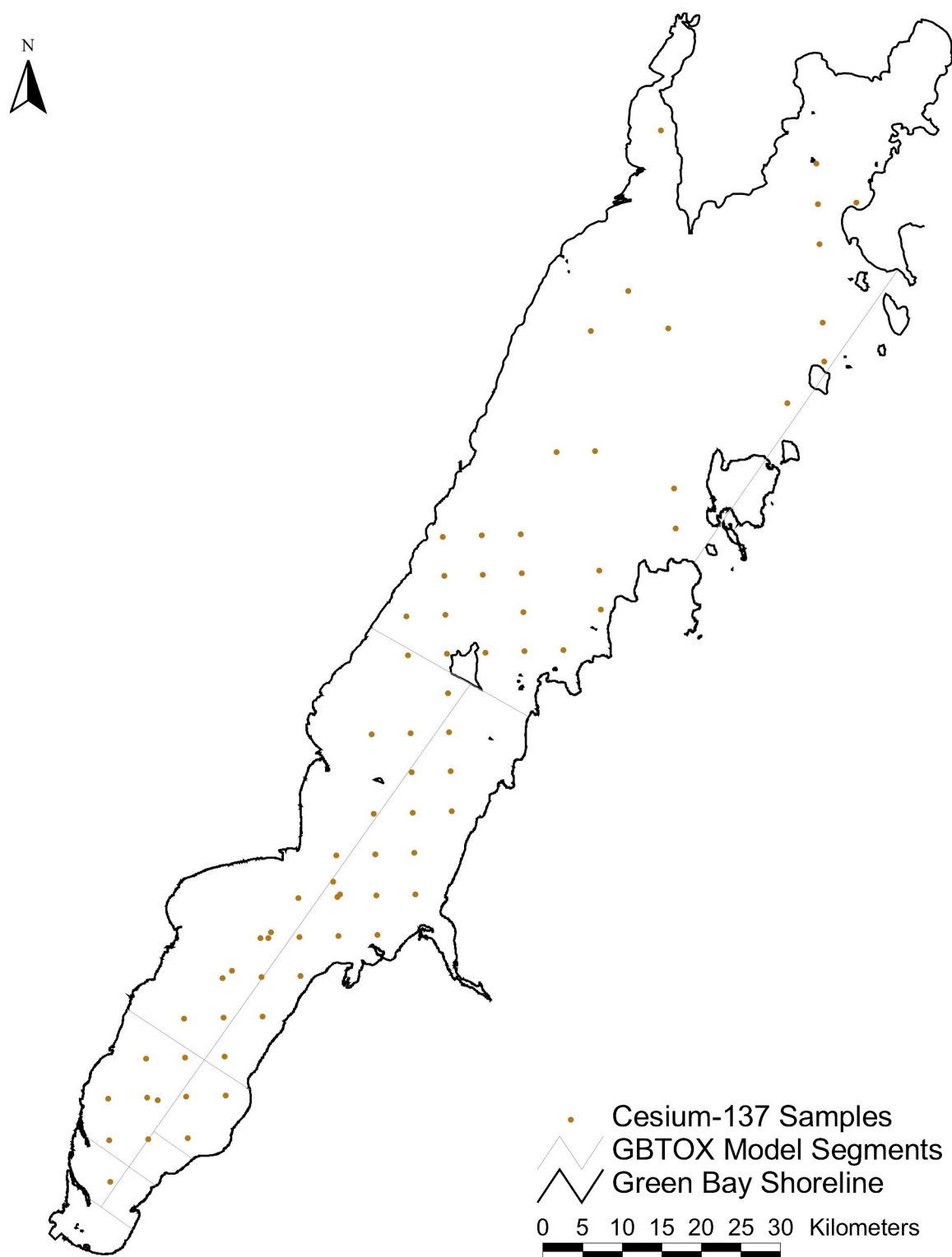


Figure 4-4. Cs-137 sample locations.



Figure 4-5. Pb-210 sample locations.

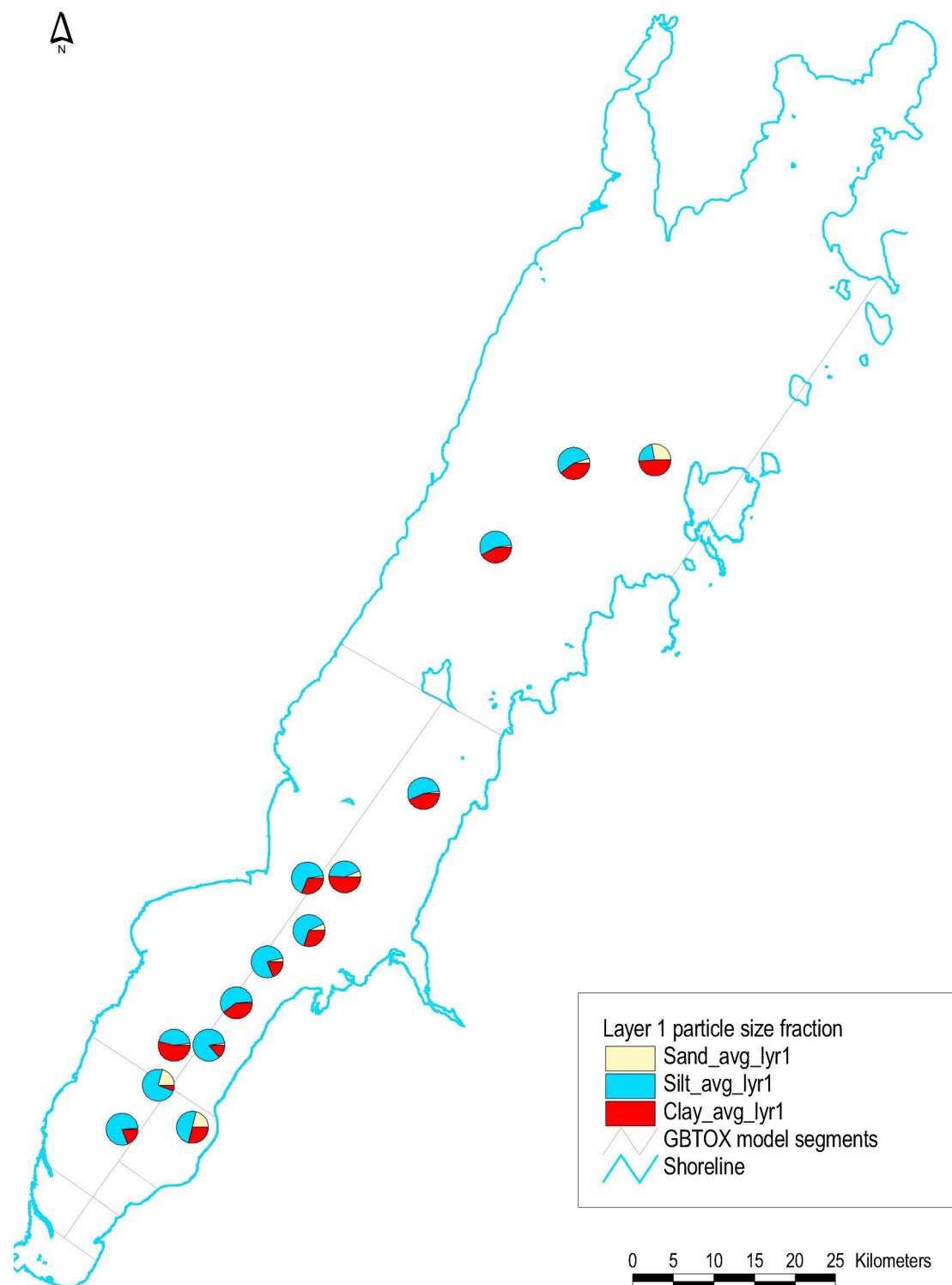


Figure 4-6. Particle size distribution and sample locations, Layer 1.

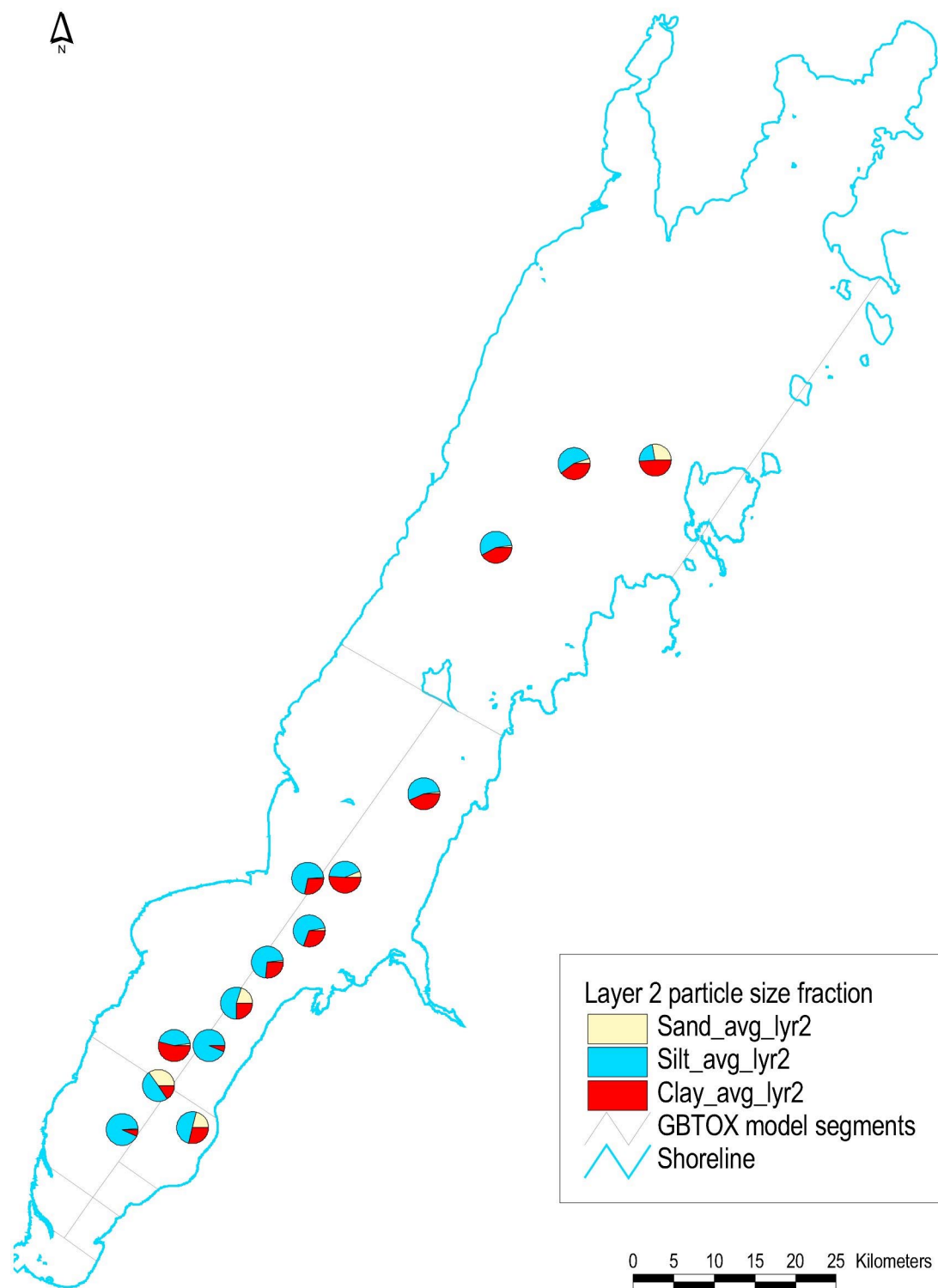


Figure 4-7. Particle size distribution and sample locations, Layer 2.

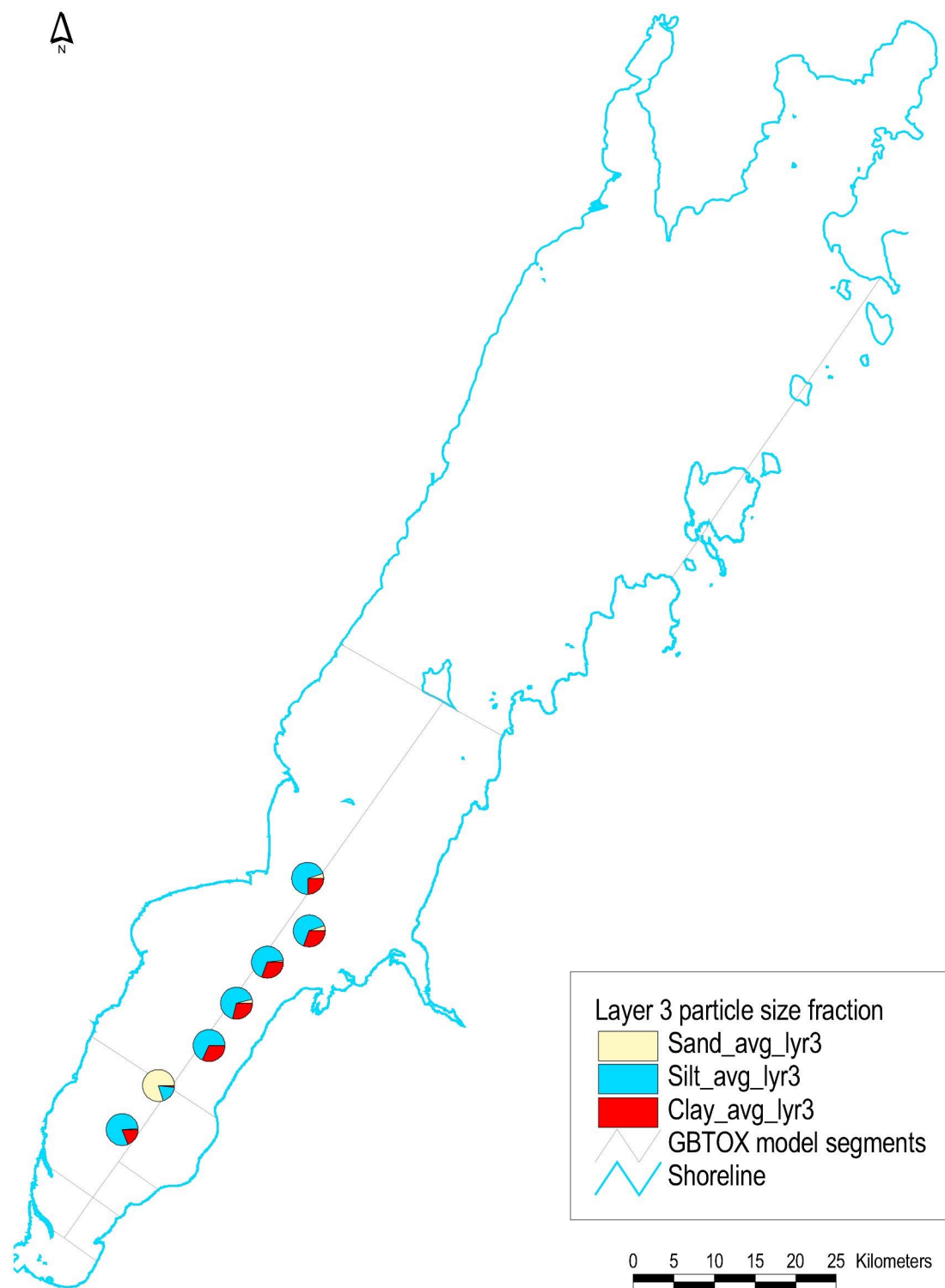


Figure 4-8. Particle size distribution and sample locations, Layer 3.

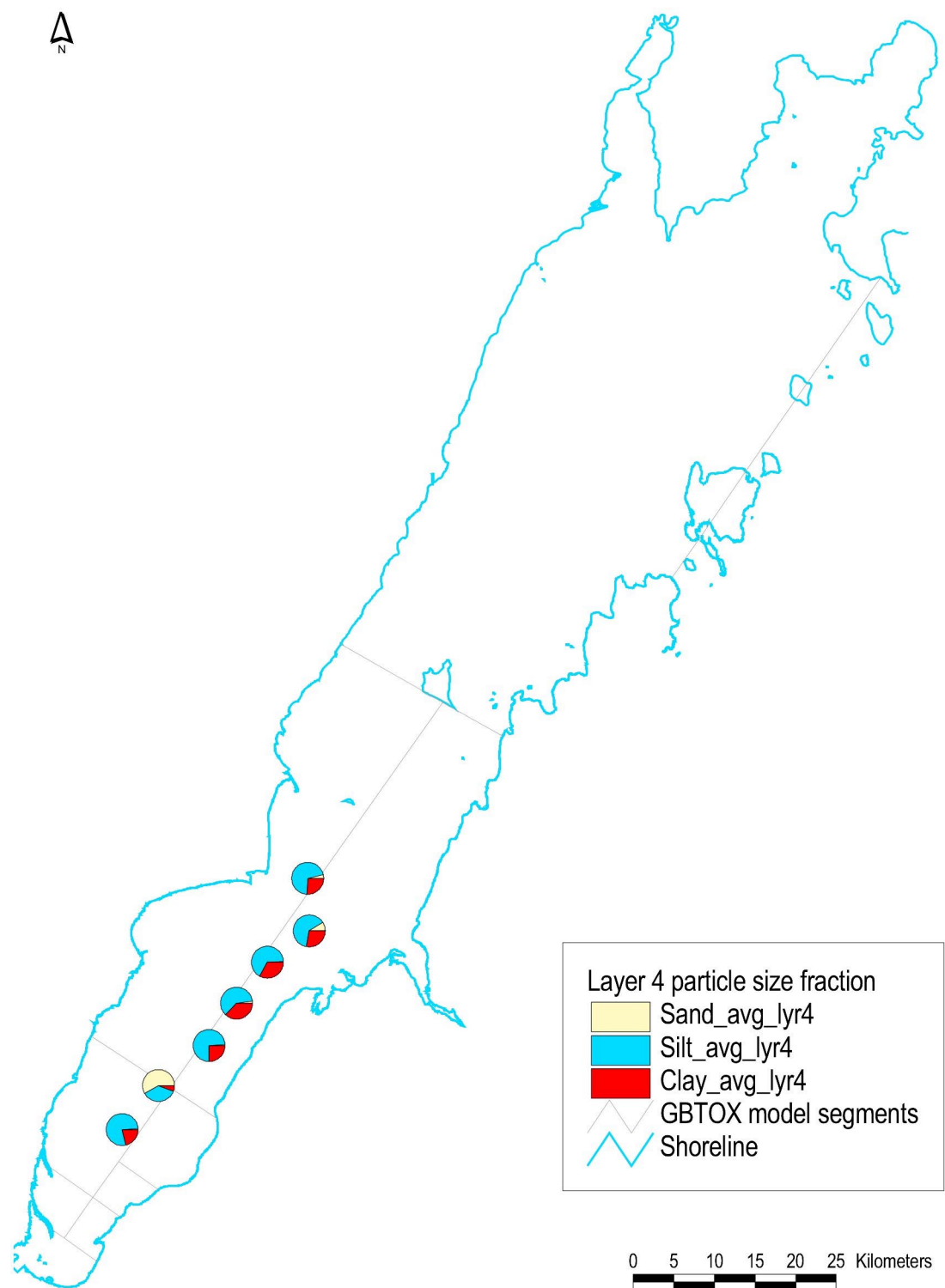


Figure 4-9. Particle size distribution and sample locations, Layer 4.

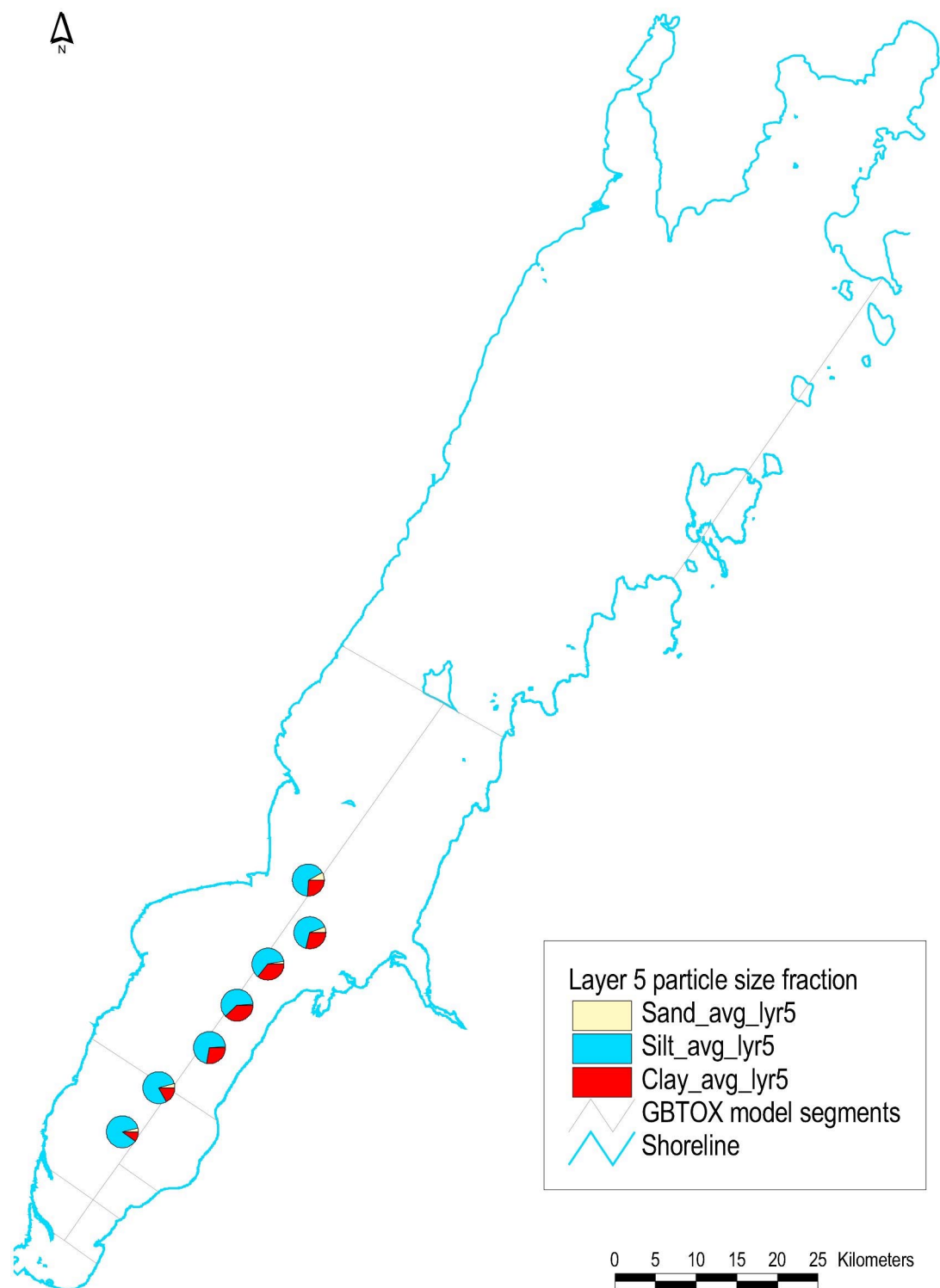


Figure 4-10. Particle size distribution and sample locations, Layer 5.

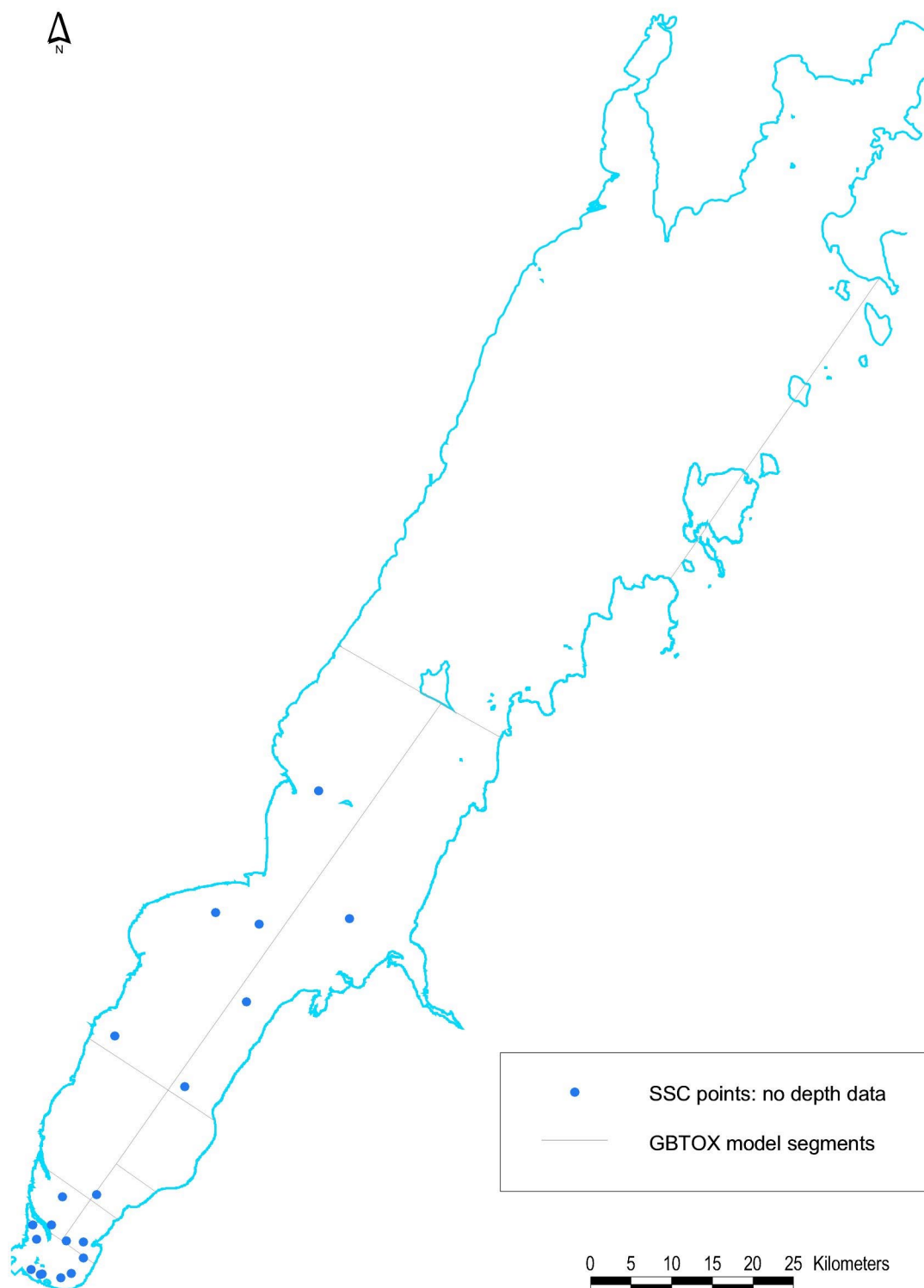


Figure 4-11. Location of particle size distribution samples without depth information.

4.5.2. ISOLATING DATA POINTS

The ARC/INFO IDW tool allows the user to choose between two basic options for selecting observed points that will influence any particular estimated value. When using the first option, the user specifies a minimum number of data points and a radius of influence. All observed data points within that radius will be used to interpolate the value. However, if the minimum number of points is not satisfied, the radius is expanded to include more distant points until the minimum number of points is obtained. With a sufficiently high minimum number of points, this method allows most or all of the study area to have interpolated values. This method was rejected for the Green Bay interpolation because it allows very distant points to have an influence where no relationship may be expected. When using the second option, the user specifies a maximum radius and a maximum number of observed data points to be used for interpolation. If the radius contains more than the maximum number of points, only the nearest points will be used. This second method was used for the interpolation of Green Bay sediment bed properties. The maximum number of points was set at a value sufficiently high such that no data would be rejected on the basis of number of data points used for interpolation. Thus, all data points within the specified radius contribute to the computation of an interpolated value.

4.5.3. RADIUS OF INFLUENCE

The radius of influence r helps determine how many data points come into use to interpolate any particular value. It also determines how much of the study area is interpolated. Any location beyond the radius distance from all data points will not be interpolated and is assigned a null value. The selected radius also determines how much actual interpolation occurs. If it is small, fewer points will influence interpolated values, and values of nearest data points will dominate. As the radius is increased, the influence of a known data point is extended far from its location.

The purpose of the interpolations is to infer the horizontal and vertical distributions of Green Bay sediment bed properties from a limited number of data points. As the radius increases, the area and volume of sediment for which properties are inferred increases. In general, interpolation error also increases as the radius increases. The resulting tradeoff between coverage and error depends upon the spatial and numerical distributions of data. In section 4.5.4, this tradeoff is quantified for the sediment bed properties interpolated.

4.5.4. OPTIMAL EXPONENT AND RADIUS COMBINATION

One way to determine the “best” map is to empirically verify the results (Berry, 1997). This process involves generating several alternate maps using different combinations of interpolation parameters (or different interpolation techniques) and then testing the results against a set of known measurements. In order to determine the optimal combination of IDW parameters for interpolating Green Bay sediment bed properties, a series of test interpolations were produced and analyzed.

Selection of the IDW exponent and radius combination was based on three objectives: maximum coverage, maximum accuracy (minimum error) of interpolation, and consistency of method for all variables interpolated. Tradeoffs arise in fulfilling these three objectives. For example,

accuracy of prediction may be greatest at a radius that provides less than 100% coverage, and may be achieved with different IDW parameters for different environmental variables. In order to satisfy the third objective, a common set of values of IDW parameters was used for all interpolations. These values were selected by examining the tradeoff between accuracy and coverage for each variable interpolated. PCB concentration was treated as the most important variable for assessing the accuracy of interpolations. The methods for estimating accuracy and coverage are discussed below, and the results that were used to select the IDW parameters are also shown and discussed.

To evaluate accuracy, a “leave one out” strategy was employed to test parameter combinations. This method, which is routinely employed in choosing interpolation parameters (Shafer and Varljen, 1990), is often called “jackknifing.” In this study, each observed sample point was removed from the data set one at a time and interpolations were performed with combinations of exponents and radii. Interpolation results were compared to the observed values in order to assess interpolation error. The more accurately a parameter combination reproduces observed values, the more attractive it is for interpolating sediment bed properties throughout the study area. This procedure is often used as an exploratory technique to formulate models to better use and conform to observations (Davis, 1987).

Data for the 0-2 cm sediment layer were used to test interpolation parameters. Tested exponents were $n = 1, 2, 3, 4$, and 5 . Tested radii were $r = 5,000, 6,000, 6,500, 7,000, 7,500, 8,000, 8,500, 9,000, 10,000, 15,000$ and $20,000$ meters. At least twenty combinations of parameters were used to perform interpolations for each jackknifed data layer.

The residuals for each data point location were calculated by subtracting the observed value from the interpolated values. The closer a residual is to zero the better the estimation. No attempt was made to minimize residuals for specific data points. Instead, an overall measure of IDW parameter combination effectiveness was obtained from the average absolute residual and from the root mean square (RMS) error (calculated by obtaining the square root of the average of the squared residual values).

Figures 4-12, 4-13, and 4-14 show RMS errors as functions of the weighting exponent and the radius for PCB concentration, total organic carbon, and dry bulk density. Minimum values of RMS for each of these variables occur between radii of 6,000 and 8,000 meters. For each variable, error is minimized at an exponent 2. Figure 4-12 shows that for radii exceeding approximately 10,000 meters, the errors associated with exponents of 1 and 2 exceed the error associated with larger exponents. This reflects the fact that the largest radii permit averaging of data from distant spatial clusterings, which may differ greatly in magnitude. Higher exponents reduce the weight attached to distant points, so they can outperform lower exponents when the radius is large. However, the lowest RMS error of PCB prediction was achieved for radii of 7,500-8,000 m and an exponent of 2.

More complete residual analysis results are presented in Appendix A. Included in those results are normalized residual indexes, which allow comparison of residual results among interpolated properties. The index is calculated by dividing the absolute residual by the average of the actual observed values (Berry, 1995).

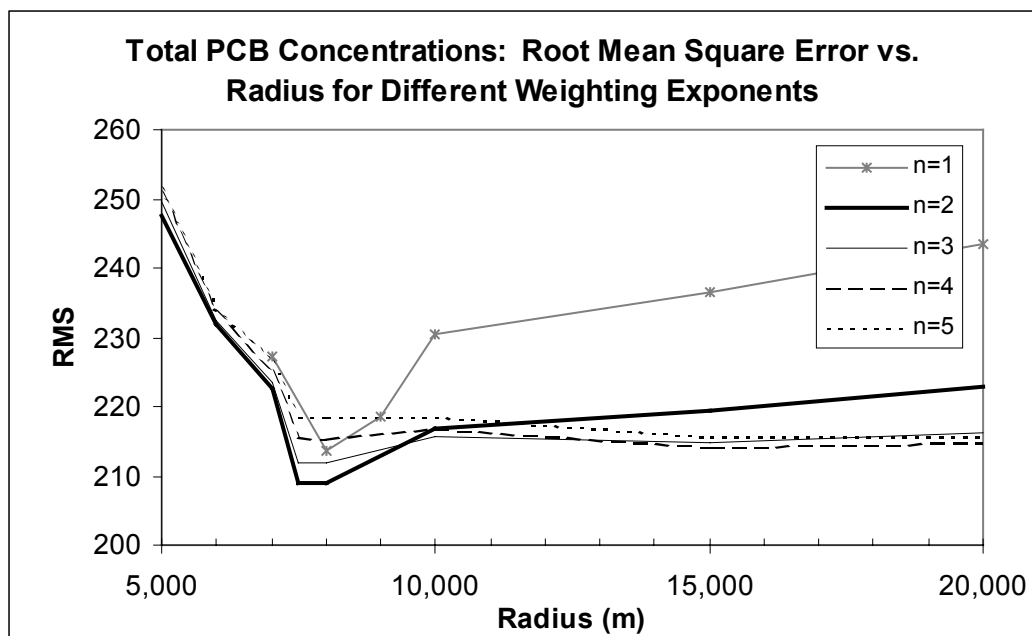


Figure 4-12. RMS error for PCB concentration (ug/kg).

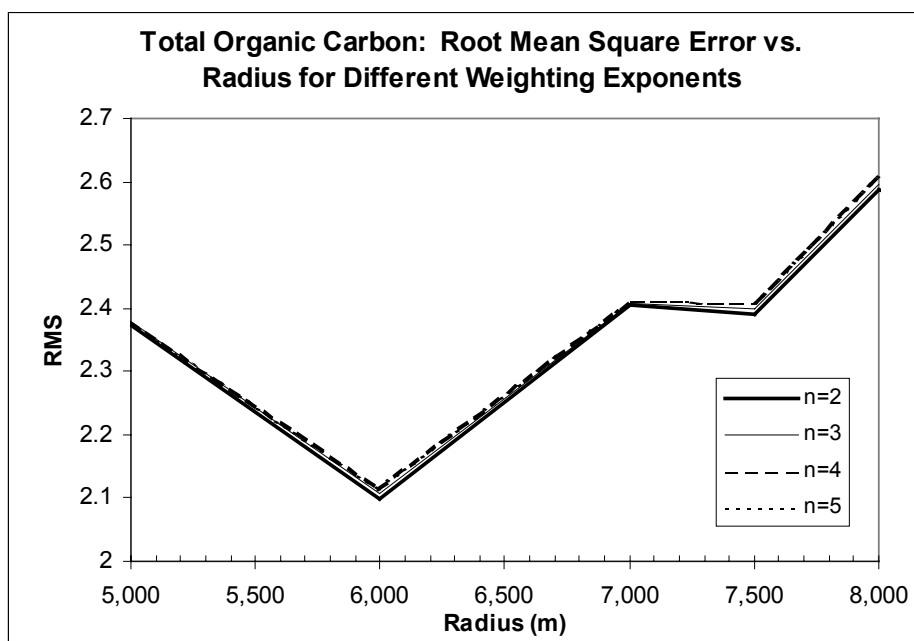


Figure 4-13. RMS error for total organic carbon (%).

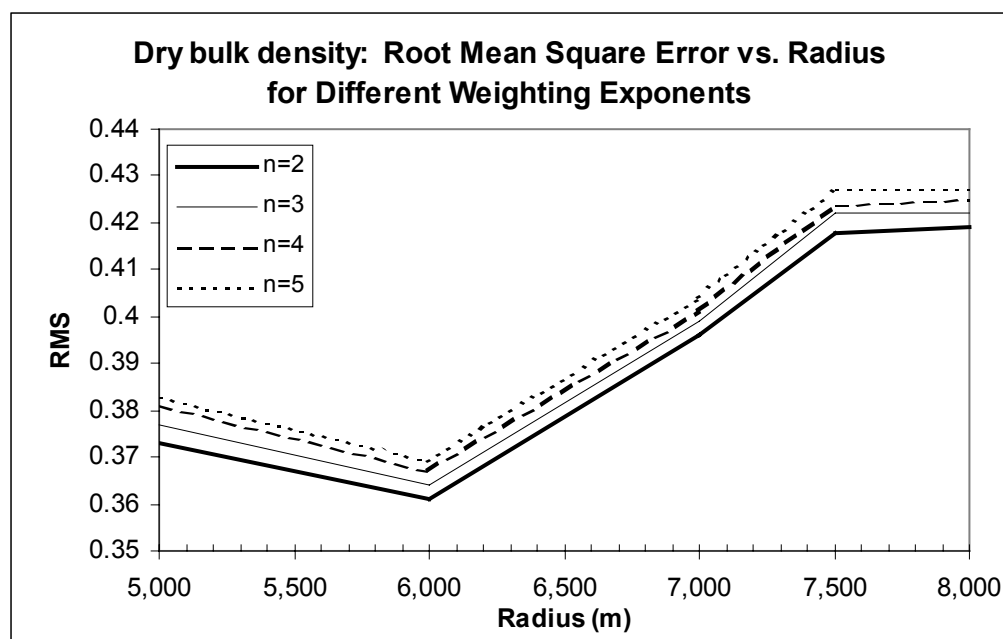


Figure 4-14. RMS error for dry bulk density (g/cm^3).

For PCB interpolations, the combination of $r = 7,500$ meters and $n = 2$ had the lowest average absolute residual. The lowest RMS was obtained by the combination $r = 8,000$, $n = 2$, followed closely by $r = 7,500$, $n = 2$. For TOC and bulk density, both average absolute residual and RMS error are minimized at $r = 6000$ m and $n = 2$.

Coverage of bay area by different radii was analyzed. For this analysis, a bed mask intended to approximate regions of the bay where “cohesive” sediments occurs was considered. (See Section 4.5.5 for discussion of interpolation barriers and the “cohesive” sediment bed mask.) Within the GIS, circular buffers were created around each PCB data point. The proportion of Green Bay “cohesive” sediment area covered by the overlapping buffers was measured for each radius. Results are shown in Figure 4-15 and Table 4-2. A 4,000 m radius covers only 74% of the “cohesive” area. A radius of 15,000 m covers virtually all of the “cohesive” area. Increasing the radius increases coverage. For example, increasing the radius from 4,000 m to 8,000 m increases the covered area by 20%. Increasing the radius another 4,000 m, from 8,000 m to 12,000 m, only increases the covered area by an additional 5%. However, dependent on the value of the weighting exponent, increasing the radius of influence can affect the accuracy of interpolation results. There is therefore a tradeoff between increasing radius of influence and interpolation error.

A large majority of data suitable for use in the interpolations originated from Green Bay Mass Balance Study efforts. The sample locations for that study were laid out on a 5-kilometer grid. The diagonal distance across a square with a GBMBS location at each corner is about 7.1 km. Therefore, an IDW radius of at least 7,100 m is needed for “communication” among neighboring sample points as sediment property values are interpolated.

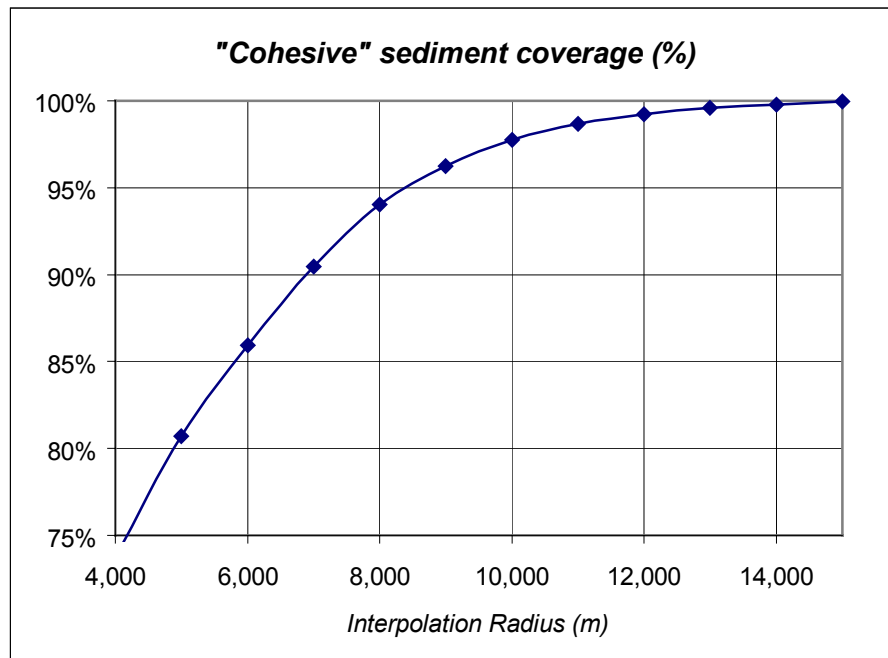


Figure 4-15. Extent of surface area coverage with radii around PCB sample locations.

Table 4-2. Extent of surface area coverage with radii around PCB sample locations.

Interpolation Radius (m)	Coverage of "Cohesive" Sediment Area (%)
4,000	73.7%
5,000	80.7%
6,000	85.9%
7,000	90.5%
8,000	94.0%
9,000	96.3%
10,000	97.8%
11,000	98.7%
12,000	99.2%
13,000	99.6%
14,000	99.8%
15,000	100.0%

Based on the jackknifing results, the extent of surface area coverage, and the spacing of most data points, a radius of 8,000 meters with an exponent of 2 was chosen as the optimal combination for IDW interpolation of PCB concentration. As shown in Figure 4-12, accuracy of prediction of PCB concentration increases until radius equals 7,500 m. For additional increases in radius up to 8,000 m, RMS error is roughly constant, so that increases in radius are justified by coverage gains. However, beyond 8,000 m some accuracy is lost (for an exponent of 2). Since 94% area coverage was achieved at a radius of 8,000 m, the gain in coverage from further increasing the radius was judged to be small. In particular, a radius increase from 8,000 m to 10,000 m would increase coverage from 94% to 98%. This potential increase in coverage was judged small, given that the error of predicted PCB concentrations increased by about 3%. The accuracy of predictions for TOC and dry bulk density were greatest at a slightly lower radius of 6,000 m. Based on these evaluations of the tradeoff between coverage and accuracy of PCB interpolations, and the objective of for consistent application of the interpolation approach, a radius of 8,000 m and an exponent of 2 were selected. The 8,000-meter radius and the weighting exponent of 2 were used to estimate all sediment bed properties.

4.5.5. INTERPOLATION BARRIERS

Barriers can be used in ARC/INFO and ArcView to control the extent of interpolations in several ways. Two ways used in estimation of Green Bay sediment bed properties were: 1) during interpolation calculations; and 2) as a post-processing “mask” following interpolation. In the absence of barriers during calculation, interpolation proceeds without restriction within the area delineated by observations and the radius of influence. In the presence of barriers during calculation, interpolation is restricted to those areas within the radius of influence and the “line of sight” of an observation. When used as a post-processing mask, a barrier defines the final extent of interpolation results.

During interpolation calculations, barriers can be used to represent the physical boundaries between areas that may have different characteristics. In general, it is reasonable to treat shorelines as interpolation barriers. For example, Long Tail Point in Green Bay could be treated as a barrier because it inhibits mixing in a portion of the inner bay. Since PCB presence at any location is the result of physical transport to that location, it is important to consider such physical barriers to mixing. However, it may not be reasonable to treat all shoreline features as interpolation barriers. For example, treating the shoreline of Chambers Island as a barrier implicitly enforces the assumption that mixing around the island can occur only on a direct (linear) line of sight. This assumption regarding a linear line of sight does not seem reasonable since currents around the island may not be linear (HQI, 1999). Therefore, to best reflect conditions within the bay, interpolation barriers were established in regions around shoreline features such as peninsulas and other convex portions of the shoreline. These shoreline barriers were applied during interpolation calculations.

Following interpolation calculations, barriers can also be used to represent boundaries. When used in this manner, a barrier represents a mask to delineate different zones. Results generated for areas outside of the barrier would then be removed from the final result. For example, sediments may not exist over 100% of the surface area of Green Bay. With a large radius of influence, sediment bed properties might nonetheless be interpolated into areas outside the region of sediment occurrence.

A post-processing mask delineating zones of sediment occurrence could be used to limit intermediate interpolations results only to zones of sediment occurrence. Results generated for areas outside of the barrier would then be removed from the final result. To account for such conditions, two post-interpolation barriers (bed masks) were applied to restrict interpolation results to areas of the bay where sediments are assumed to occur.

The first bed mask was intended to approximate regions where “cohesive” sediments occur based on consideration of: 1) successful sampling for PCB and/or TOC; 2) location compared to the interpretation of sediment occurrence presented by Moore et al. (1973); and 3) the sand content of samples obtained from an area. The second bed mask was intended to approximate regions of “soft” sediment occurrence based on consideration of the organic carbon content in sediments at a sample location (HQI, 1999). For reference, the sediment survey from Moore et al. is presented in Figure 4-16. The “cohesive” sediment occurrence bed mask is presented in Figure 4-17. The “soft” sediment occurrence bed mask is presented in Figure 4-18. It is worth noting that the sediment areas defined by the two bed masks are similar but do not exactly correspond as a result of the different assumptions regarding their development.

These two bed masks were used to limit interpolation results to areas where cohesive/soft sediments were inferred to exist. The total surface area of Green Bay was estimated to be 4,219 km². As delineated by the “cohesive” sediment bed mask, the sediment surface area was estimated to be 2,344 km² (55.6% of the total bay surface area). As delineated by the “soft” sediment bed mask, the sediment surface area was estimated to be 2,175 km² (51.5% of the total surface area). The area common to both masks is 1,784 km² (42.3% of the total bay surface area, 82% of the “cohesive” sediment surface area). When tabulating depth of analysis, Cs-137, and Pb-210, interpolation results were bounded to the extent of the “cohesive” sediment bed mask. When tabulating dry bulk density, PCB concentrations and mass inventories, and TOC, interpolation results were bounded to the extent of the “soft” sediment bed mask. Interpolation results that fall outside of the bounding sediment bed mask area are not included in summary computations. Therefore, estimates of total sediment volume and chemical mass inventories are applicable to less than half the total surface area of the Green Bay.

4.5.6. GRID CELL SIZE

In order to perform analysis using raster data, a uniform grid cell size must be specified. The cell size must be small enough to provide meaningful interpolation results among data points. If the cell size is very large, little or no interpolation will occur among points, and the sediment bed property estimates will be poor. Also, a coarse cell size will provide a poor representation of the shoreline, introducing inaccuracies in sediment bed property estimations on the edges of the study area. The cell size must be large enough so that GIS analysis does not take excessively long periods of time. A cell size of 100 m by 100 m was chosen for the Green Bay sediment bed property interpolations. This grid cell size provided a good resolution of shoreline features and was not burdensome for interpolation computations.

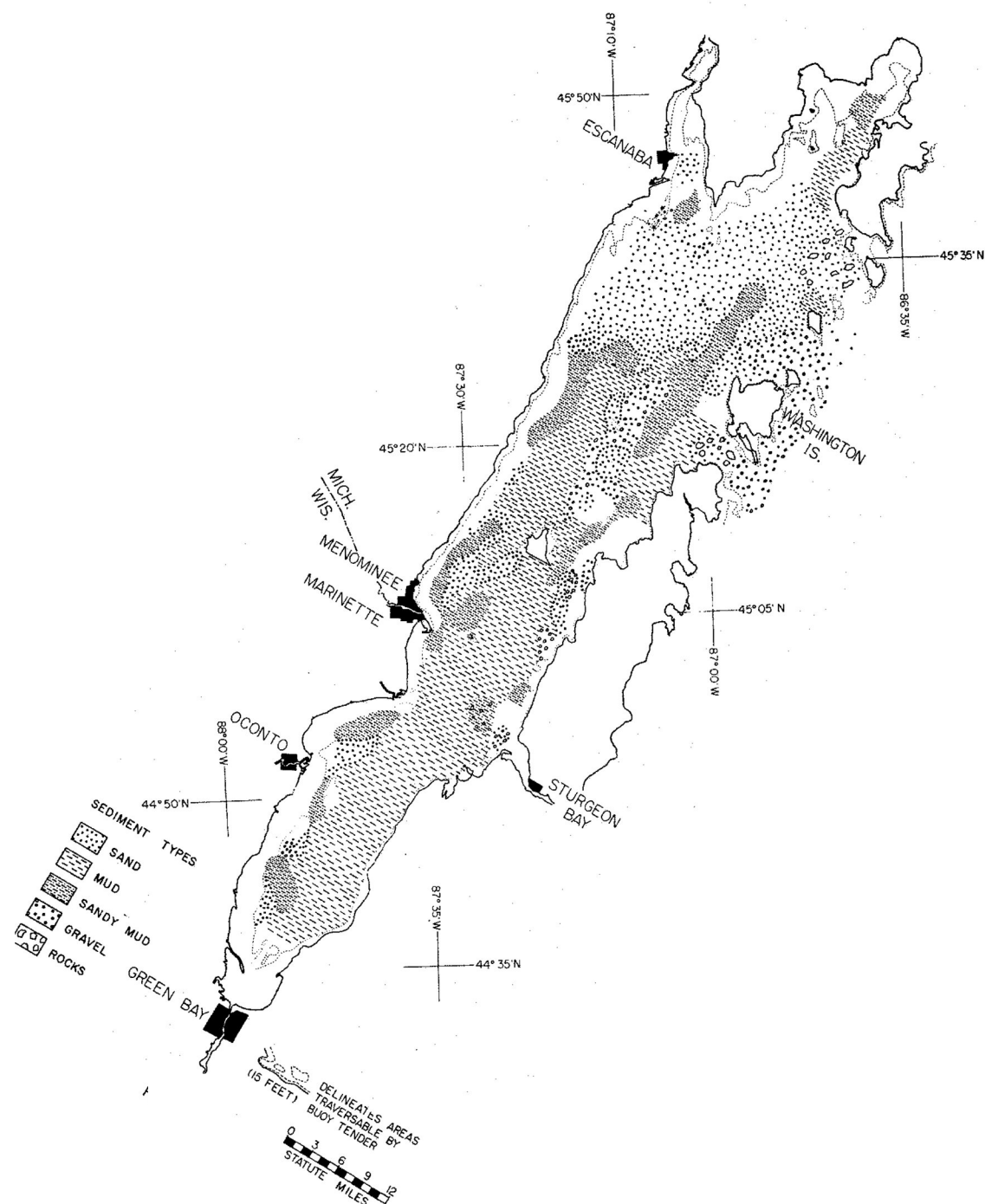


Figure 4-16. Green Bay sediment classification (from Moore et al. 1973).

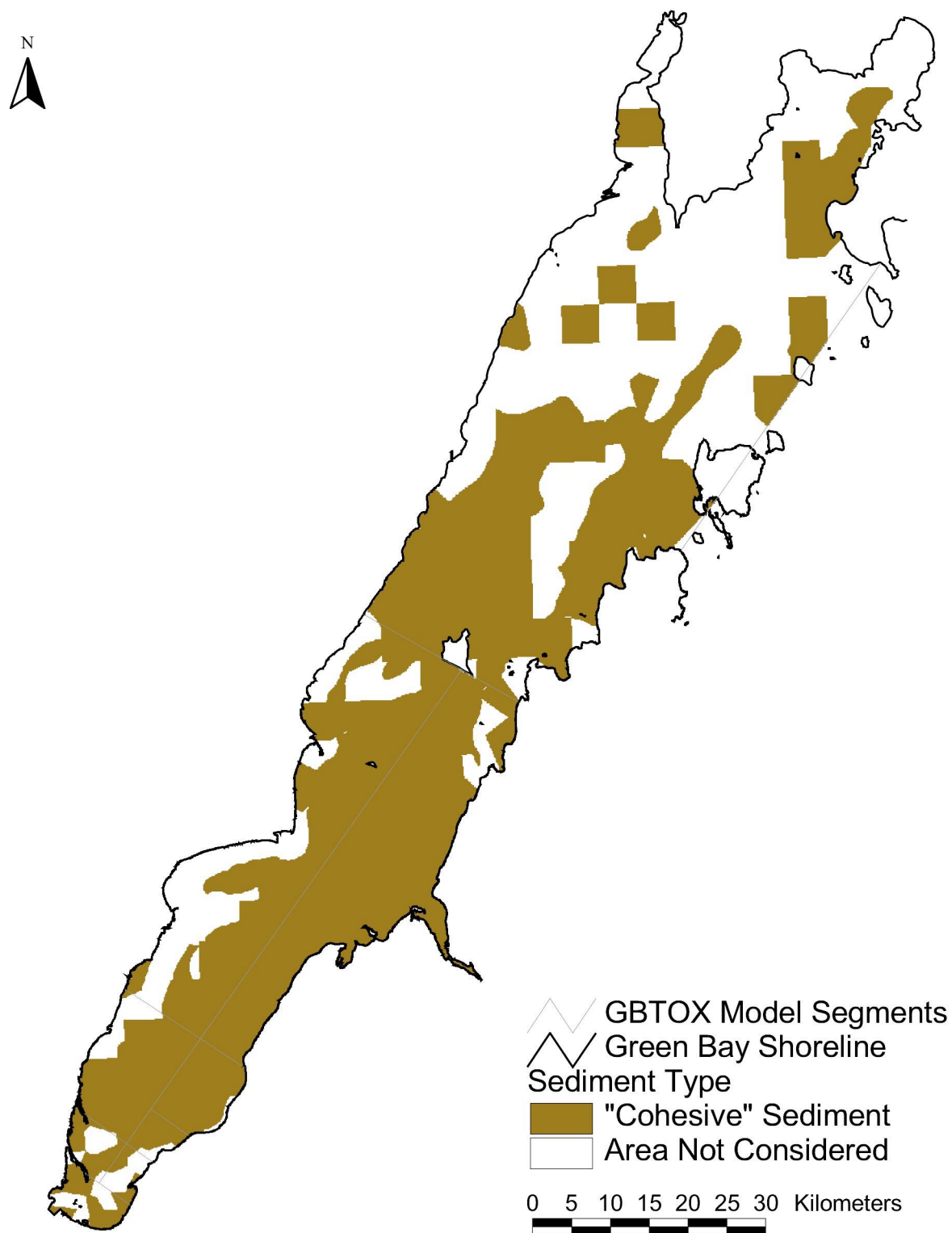


Figure 4-17. "Cohesive" sediment areas of Green Bay.

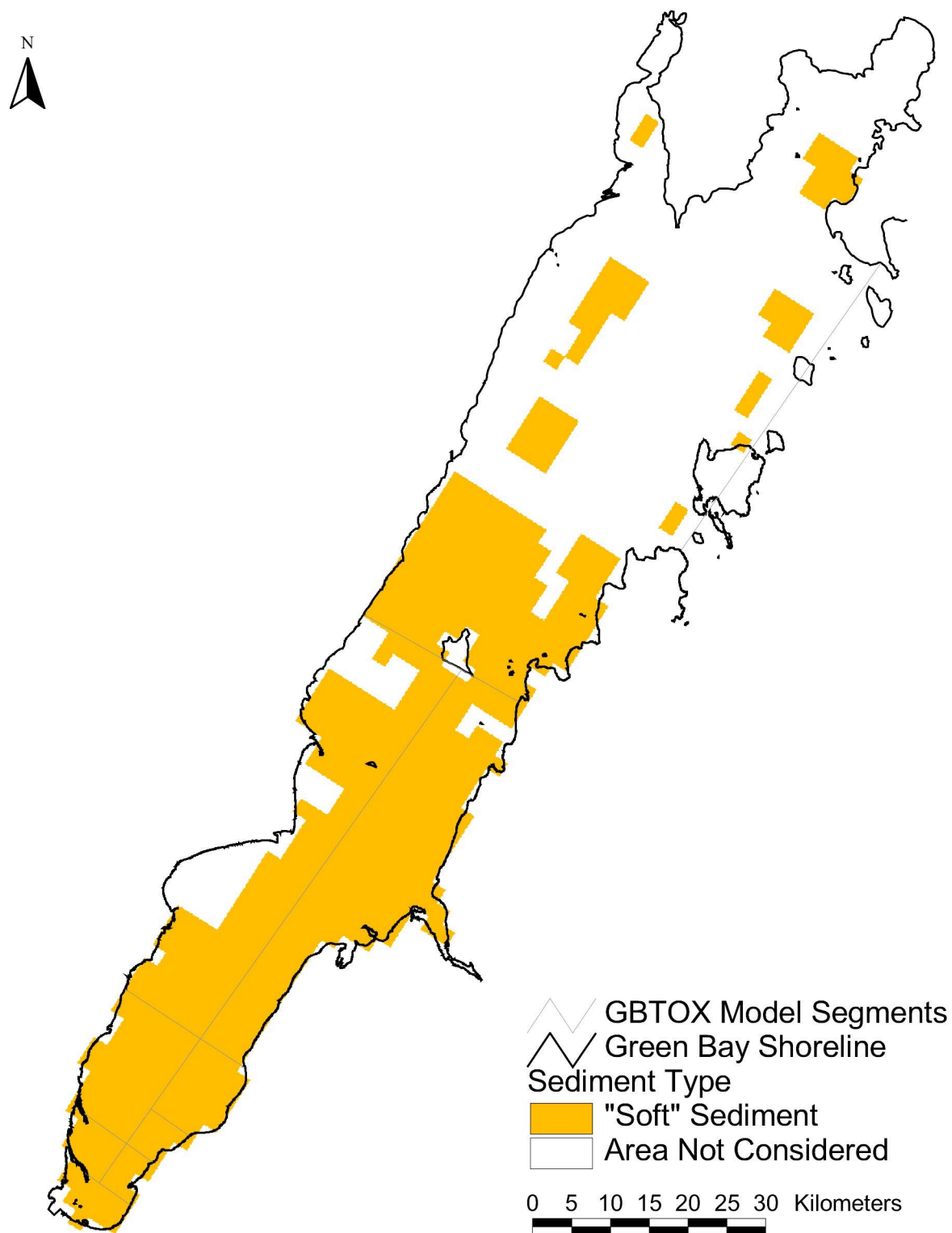


Figure 4-18. "Soft" sediment areas of Green Bay.

5.0 ESTIMATED GREEN BAY SEDIMENT BED PROPERTIES

The results of interpolation for each sediment bed property are presented in the sections that follow. For data interpolated as five vertical sediment layers, the stratification used, in distance from the sediment-water interface, was:

Layer	Depth (cm)
1	0 - 2
2	2 - 4
3	4 - 6
4	6 - 10
5	> 10

Summaries of sediment bed properties interpolation results by GBTOX model segment are presented in Appendix B.

5.1. DEPTH OF ANALYSIS (MINIMUM SEDIMENT THICKNESS)

The maximum depth for each sample was used as a surrogate sediment thickness value for the particular parameter to which it is associated. The depth of analysis was computed based from the sample collection depths of bulk density samples and interpolated across the assumed “cohesive” sediment area of Green Bay. The interpolated depth of analysis can be used as a lower bound estimate for sediment thickness since at each location sampled location sediment extended at least as deep as the deepest core slice analyzed. Bulk density depth of analysis was selected for this interpolation because, relative to other parameters such as PCBs, bulk density samples were usually collected from deeper portions of the sediment column.

Depth of analysis interpolation results, bounded to the extent of the “cohesive” sediment bed mask, are presented in Figure 5-1. Estimated average depth of analysis values for the “cohesive” sediment areas of GBTOX model segments are presented in Appendix B, Table B-1. The PCB contaminated sediment volume was estimated to be 622,353,000 m³ (see Appendix B, Table B-4).

5.2. DRY BULK DENSITY

Dry bulk density was interpolated of Green Bay for each of the five sediment layers. Bulk density interpolation results are presented in Figures 5-2 through 5-6. Estimated average dry bulk density values for the “soft” sediment areas of GBTOX model segments are presented in Appendix B, Table B-2.

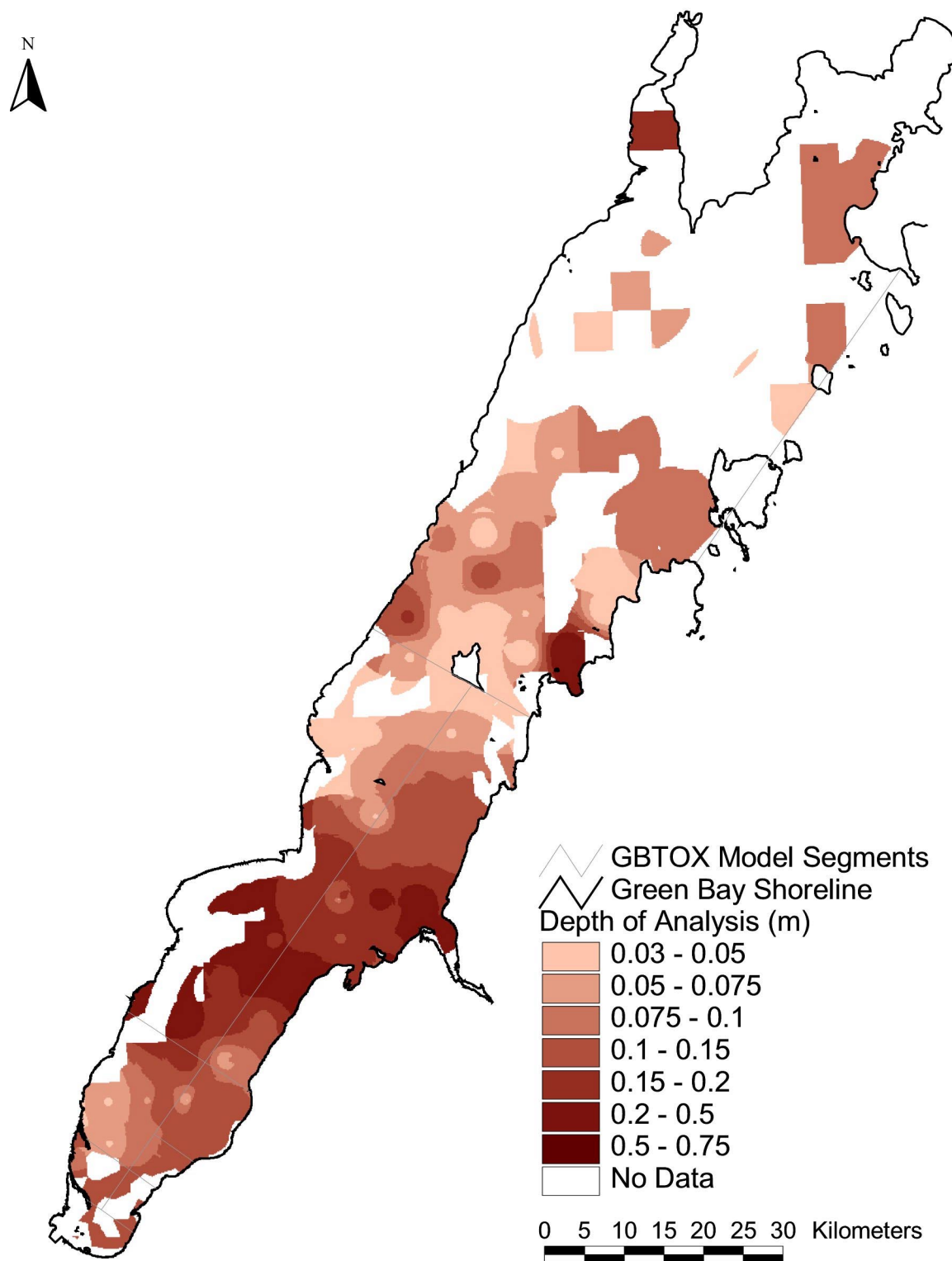


Figure 5-1. Interpolated depth of analysis (minimum sediment thickness) in "cohesive" sediment areas (m).

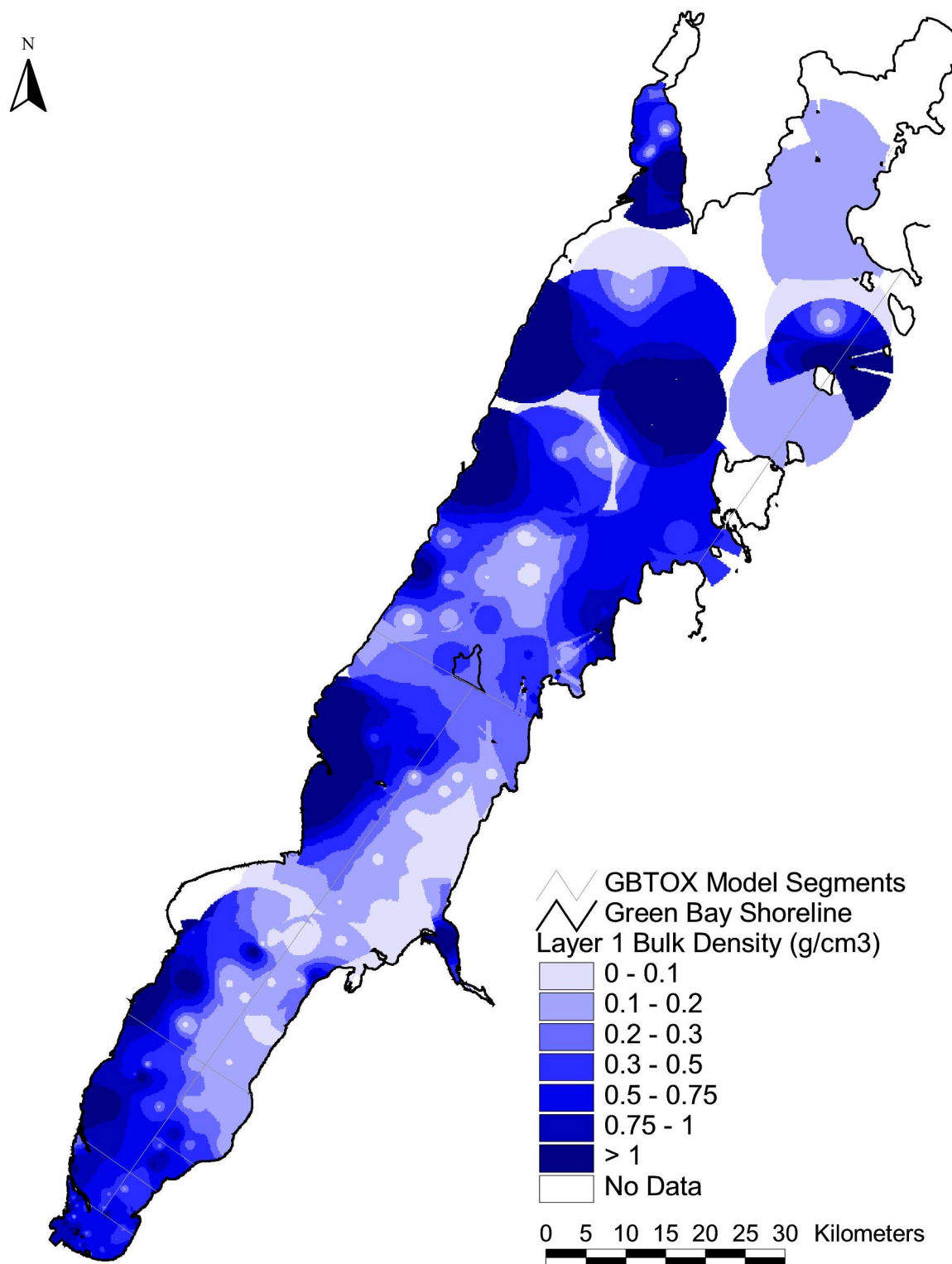


Figure 5-2. Interpolated dry bulk density, Layer 1 (g/cm³).

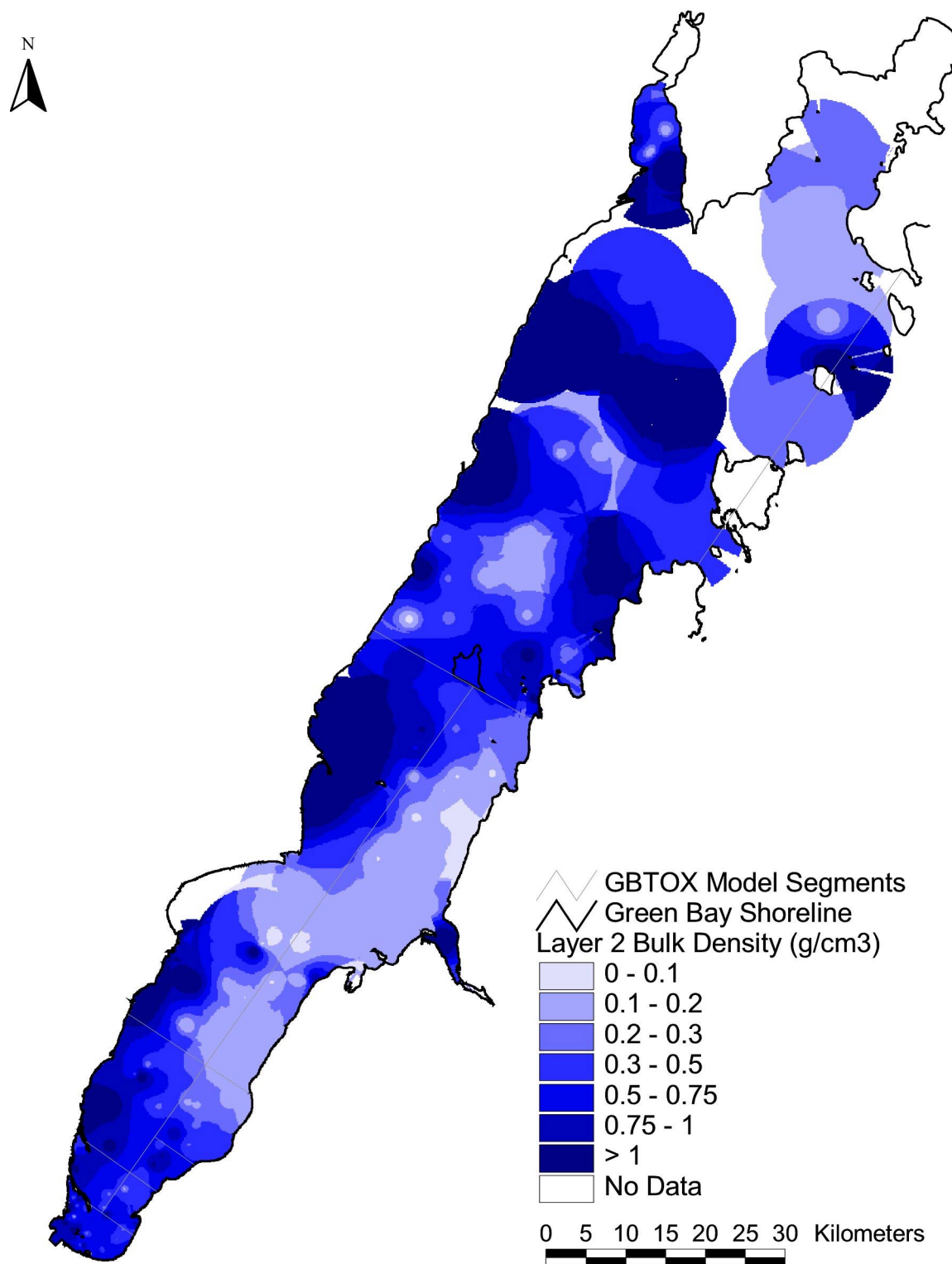


Figure 5-3. Interpolated dry bulk density, Layer 2 (g/cm³).

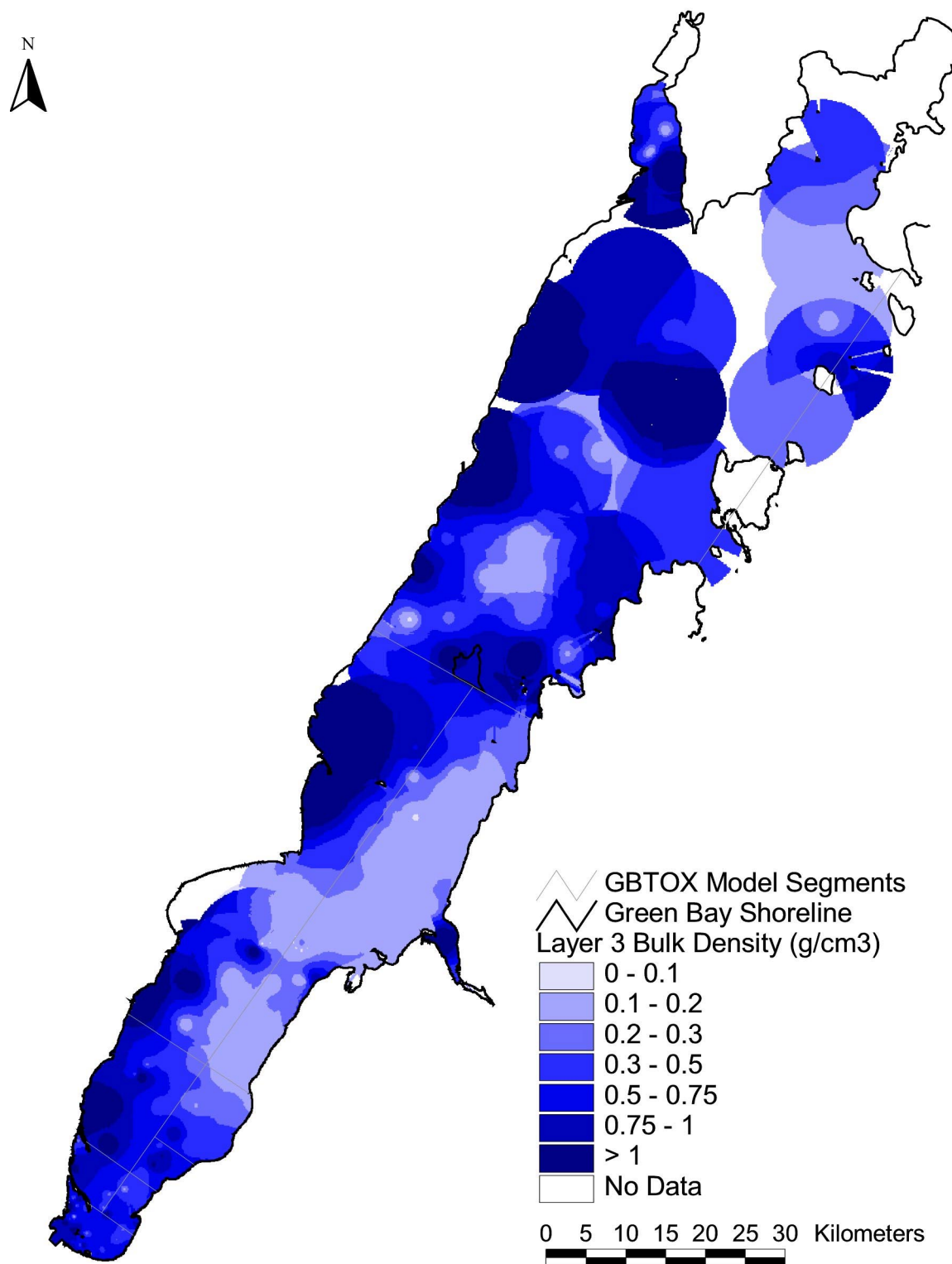


Figure 5-4. Interpolated dry bulk density, Layer 3 (g/cm³).

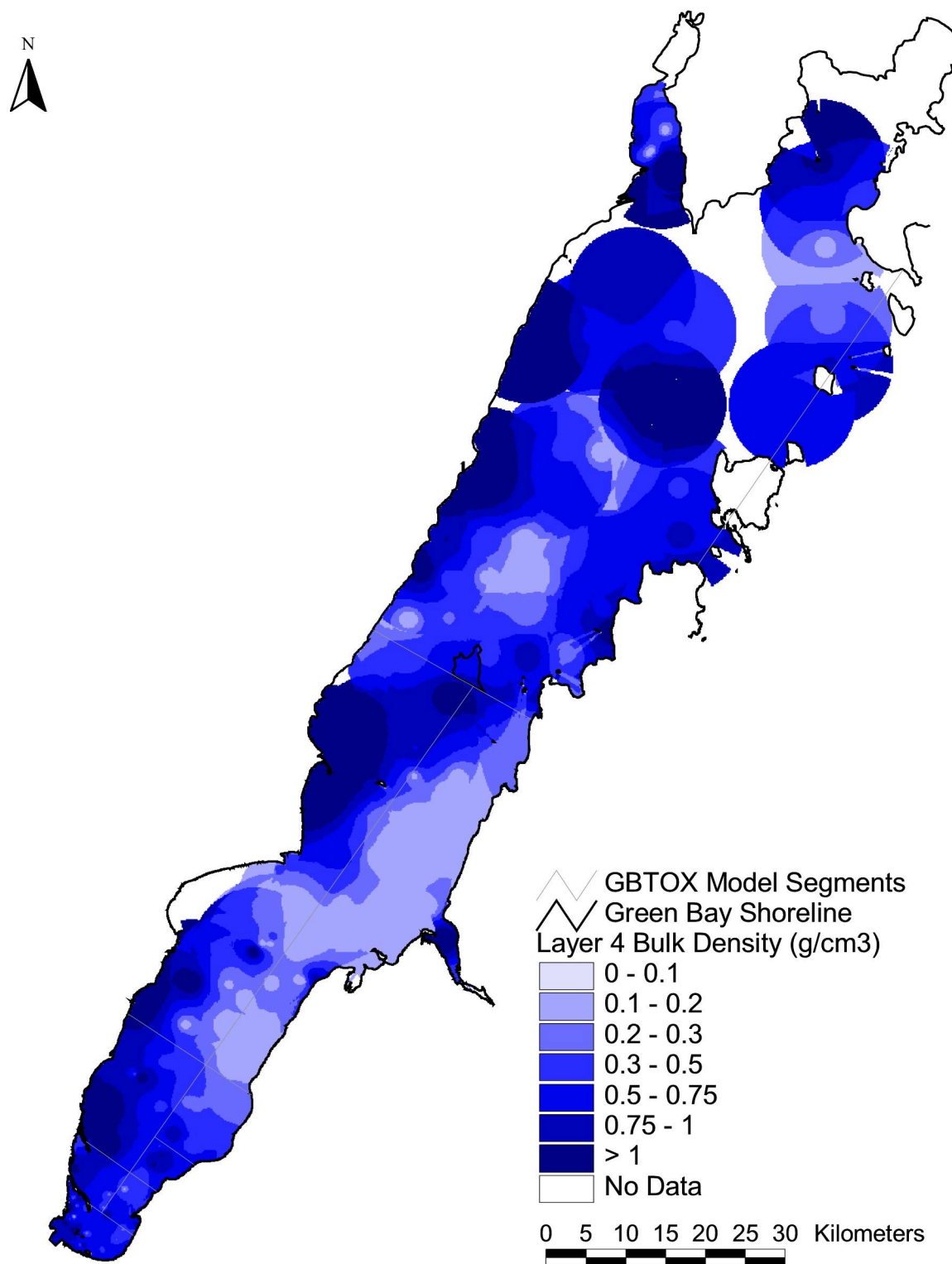


Figure 5-5. Interpolated dry bulk density, Layer 4 (g/cm^3).

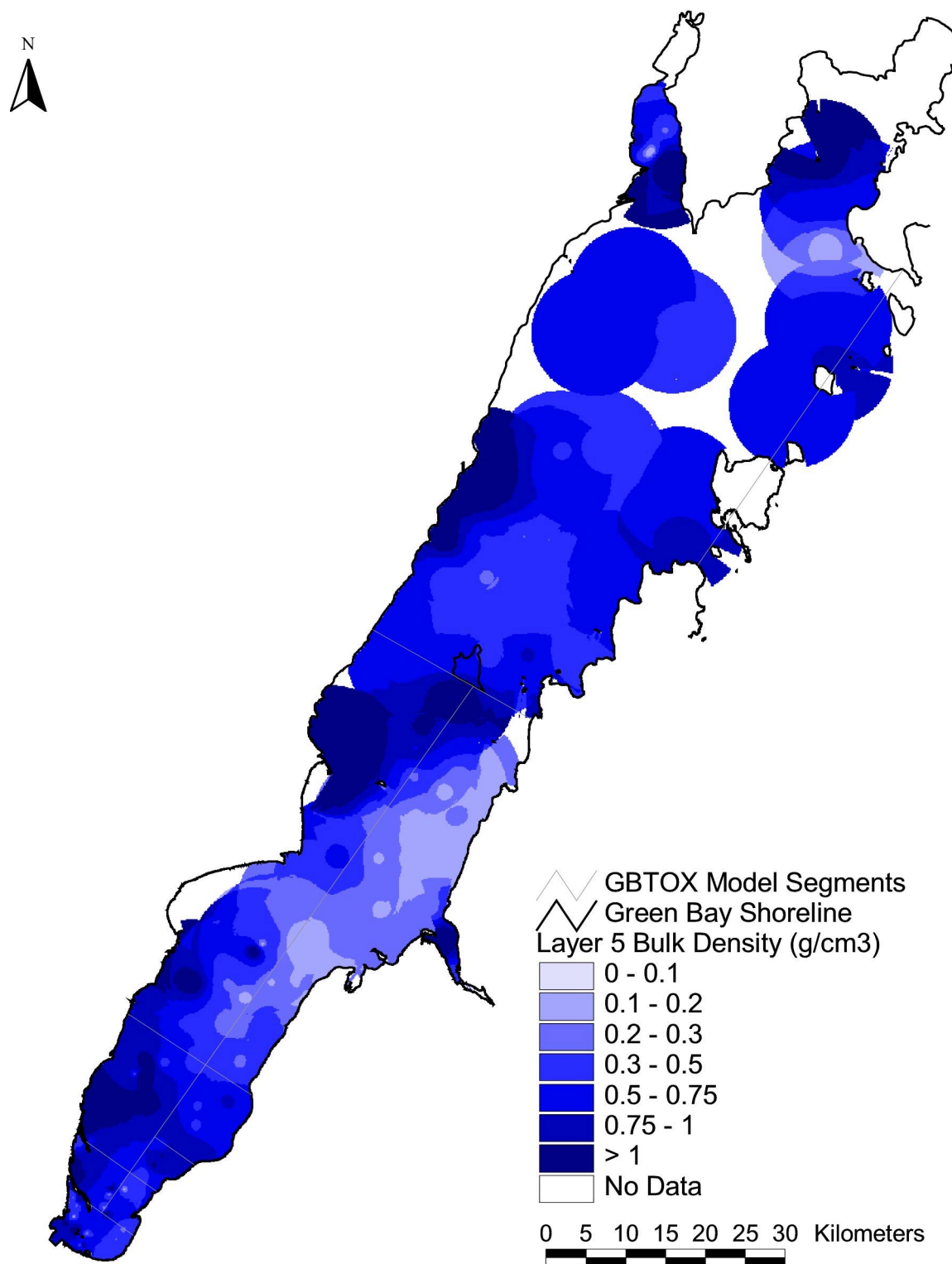


Figure 5-6. Interpolated dry bulk density, Layer 5 (g/cm³).

5.3. TOTAL PCBs

Total PCBs were interpolated for each of the five sediment layers. Total PCB concentration interpolation results for each layer are shown in Figures 5-7 through 5-11. Estimated average total PCB concentration values for the “soft” sediment areas of GBTOX model segments are presented in Appendix B, Table B-3. PCB mass inventory was estimated from bulk density and total PCB concentration interpolation results, sediment thickness, and surface area. As noted in Section 4.5.5, the surface area used in this computation was the surface area of the “soft” sediment bed mask. The PCB mass inventory was estimated to be 69,955 kg. Estimated PCB mass inventory values for the “soft” sediment areas of GBTOX model segments are presented in Appendix B, Tables B-4 and B-5.

It should be noted that PCB concentrations in the deepest core slices analyzed for PCBs were generally greater than zero. From this, it is reasonable to infer that PCBs exist at greater depths in the sediment column than the depths for which sediment samples were collected. Further, the areal extent of sediments for which the PCB mass inventory was limited to the area of the “soft” sediment bed mask. PCB contaminated sediments may also exist at locations outside the inferred area of “soft” sediment extent. For these reasons, the PCB mass inventory of 69,955 kg may be a lower bound or minimum estimate.

5.4. TOTAL ORGANIC CARBON (TOC)

Total organic carbon was interpolated for each of the five sediment layers. TOC interpolation results for each of the five sediment layers are presented in Figures 5-12 through 5-16. Estimated average total organic carbon values for the “soft” sediment areas of GBTOX model segments are presented in Appendix B, Table B-6.

5.5. Cs-137

Cesium-137 was interpolated for each of the five sediment layers. Cesium-137 interpolation results for each of the five sediment layers are presented in Figures 5-17 through 5-21. Estimated Cesium-137 values for the “cohesive” sediment areas of GBTOX model segments are presented in Appendix B, Table B-7.

5.6. Pb-210

Lead-210 was interpolated for each of the five sediment layers. Lead-210 interpolation results for each of the five sediment layers are presented in Figures 5-22 through 5-26. Estimated Lead-210 values for the “cohesive” sediment areas of GBTOX model segments are presented in Appendix B, Table B-8.

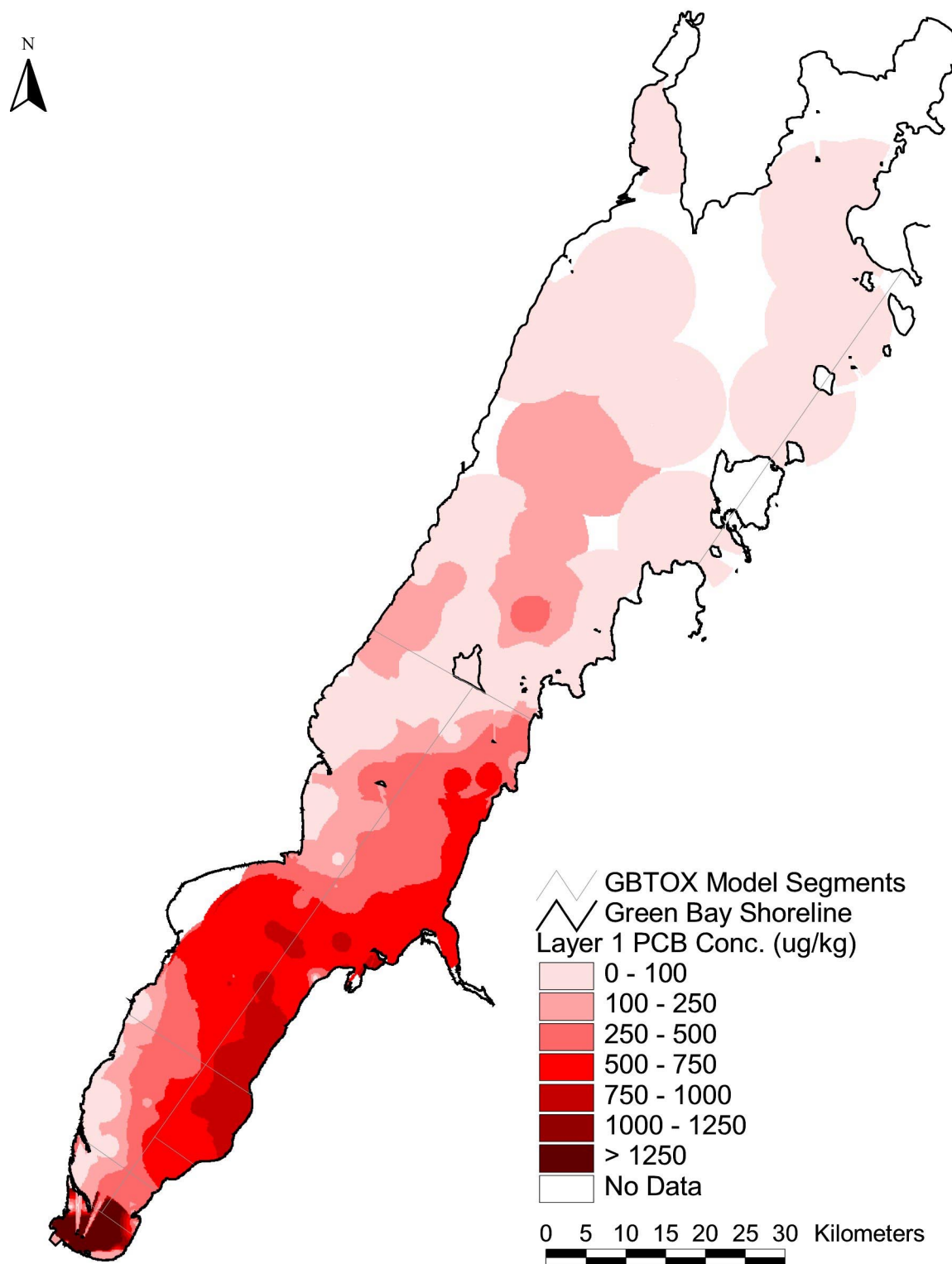


Figure 5-7. Interpolated Total PCB concentration (ug/kg) in Layer 1 (0-2 cm).

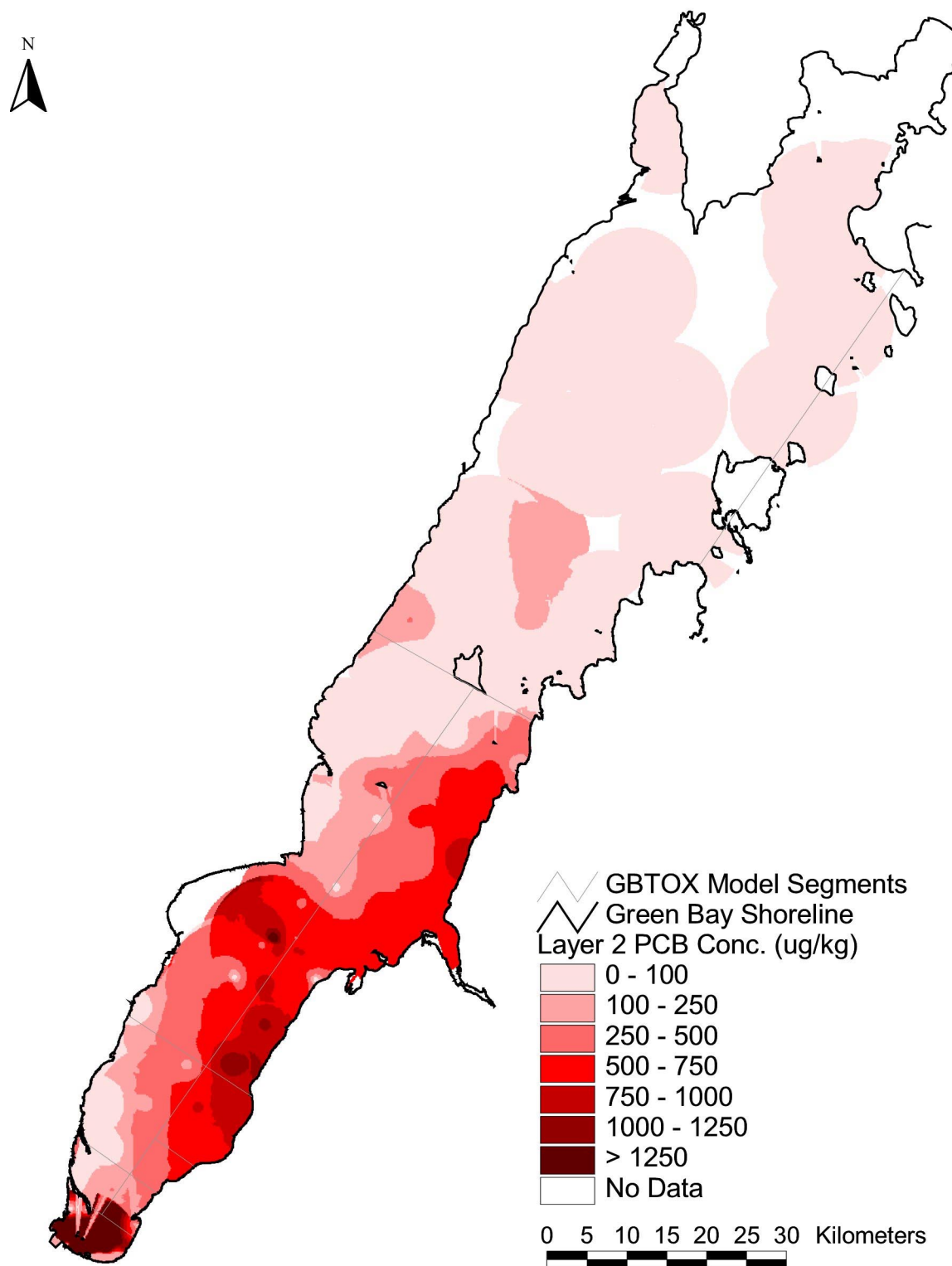


Figure 5-8. Interpolated Total PCB concentration (ug/kg) in Layer 2 (2-4 cm).

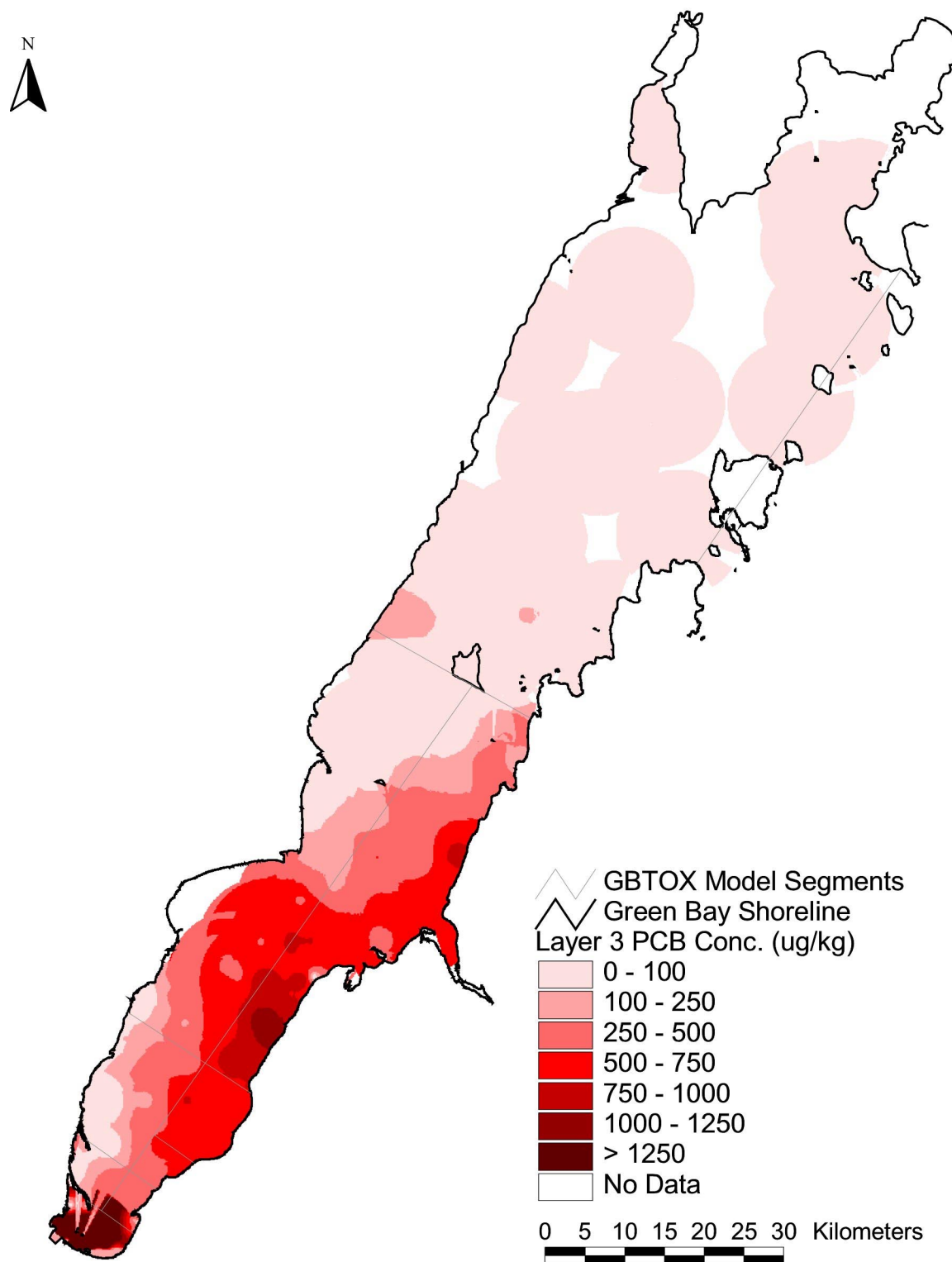


Figure 5-9. Interpolated Total PCB concentration (ug/kg) in Layer 3 (4-6 cm).

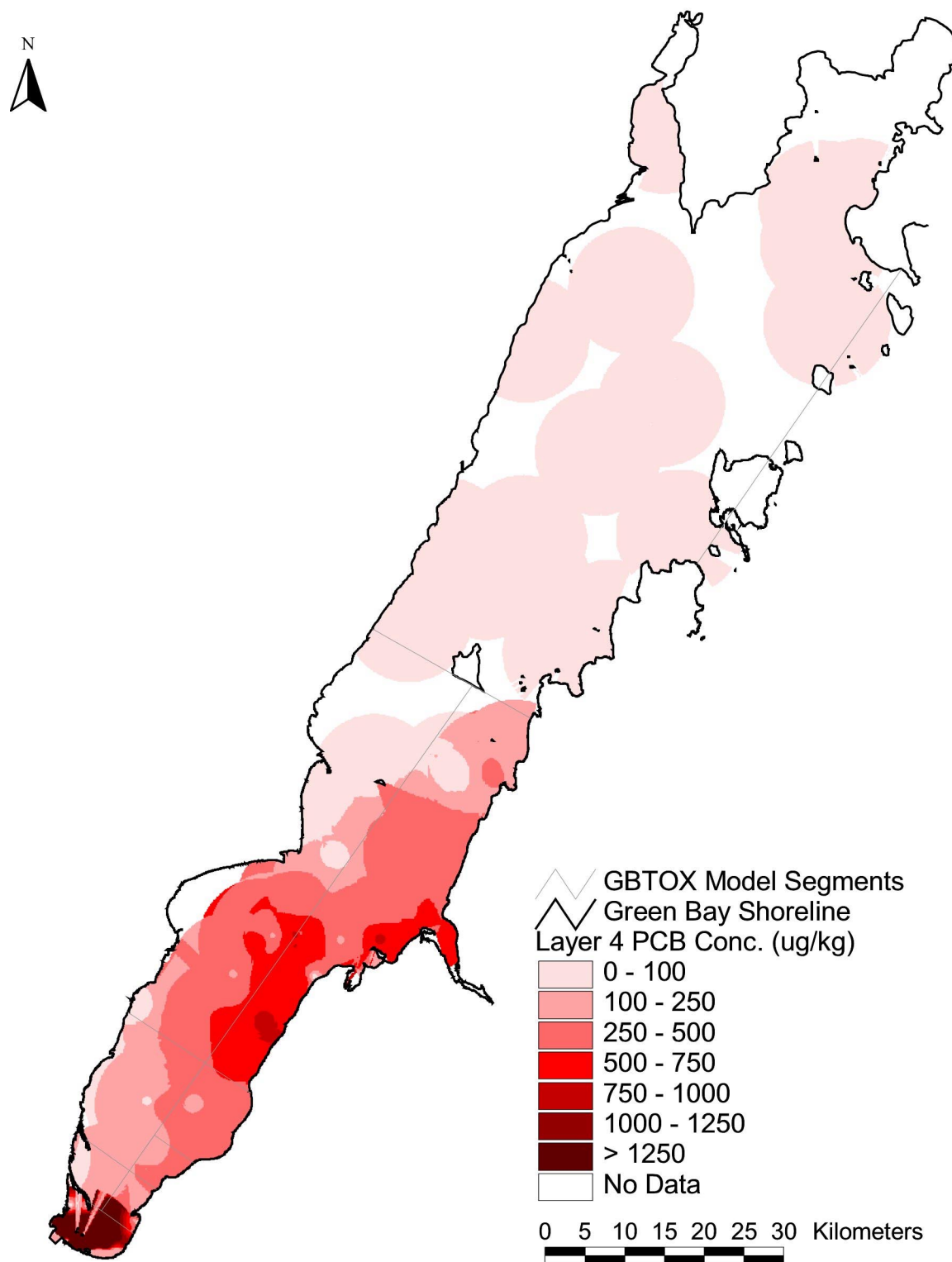


Figure 5-10. Interpolated Total PCB concentration (ug/kg) in Layer 4 (6-10 cm).

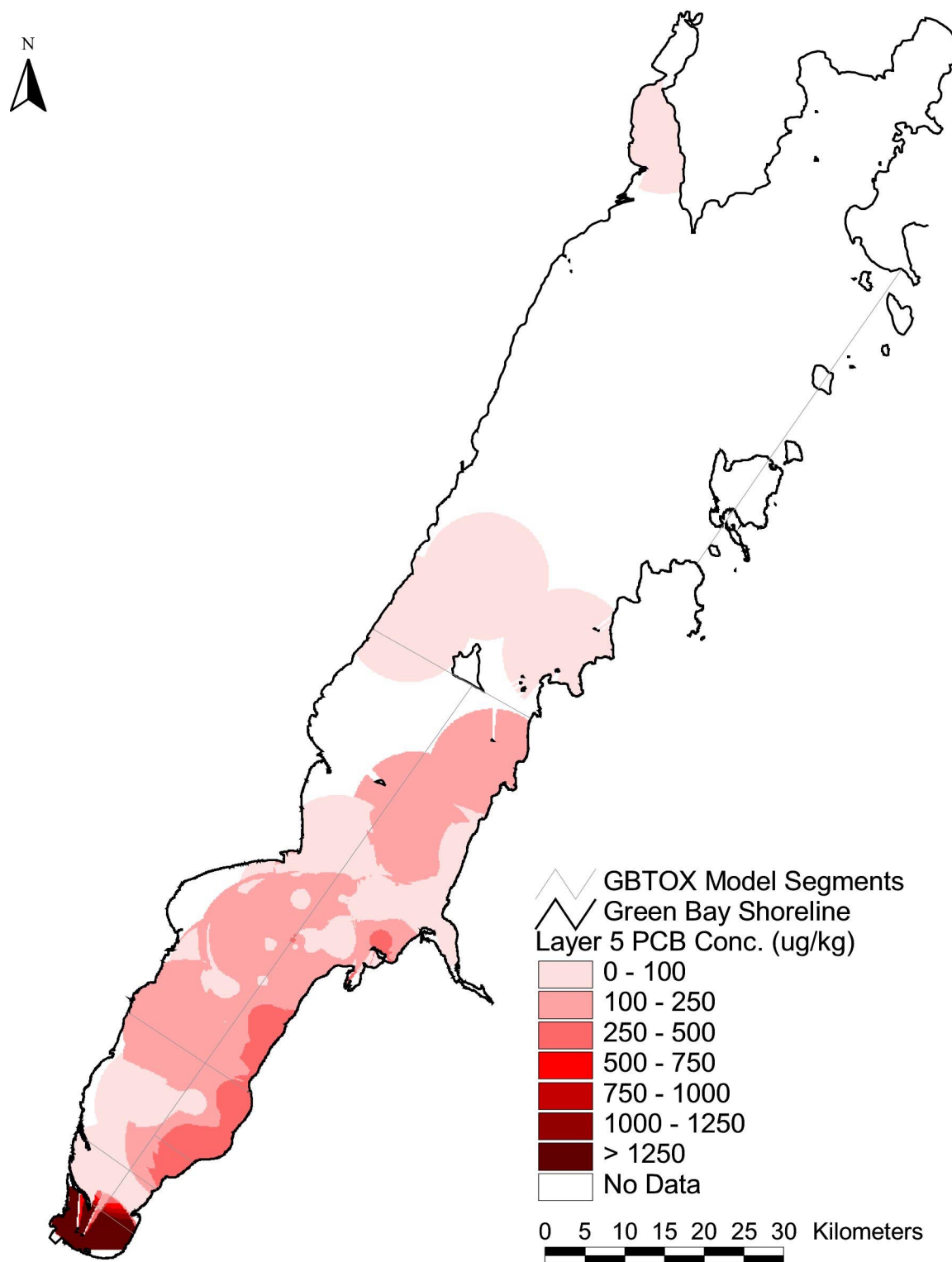


Figure 5-11. Interpolated Total PCB concentration (ug/kg) in Layer 5 (>10 cm).

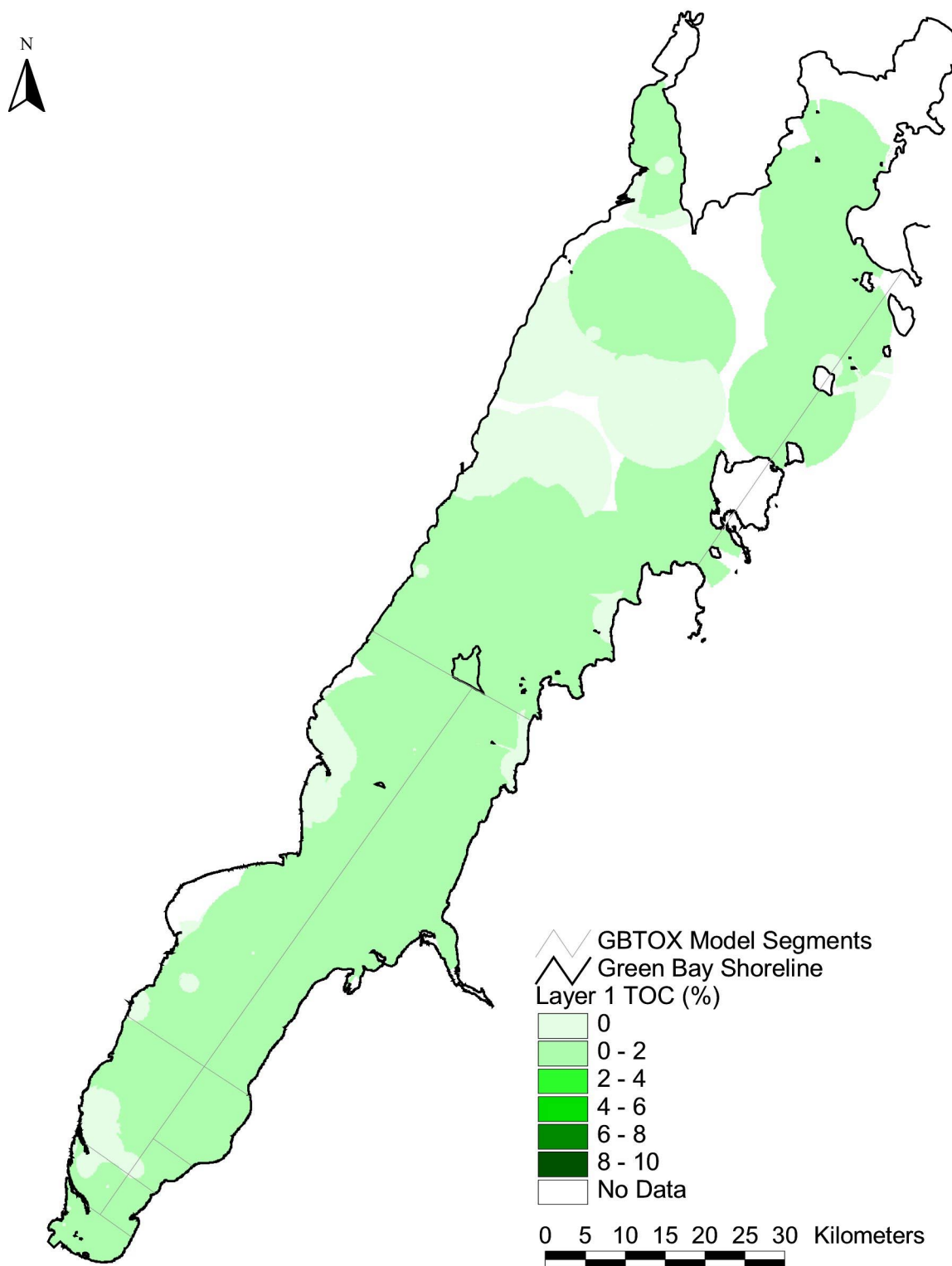


Figure 5-12. Total organic carbon (%) in Layer 1 (0-2 cm).

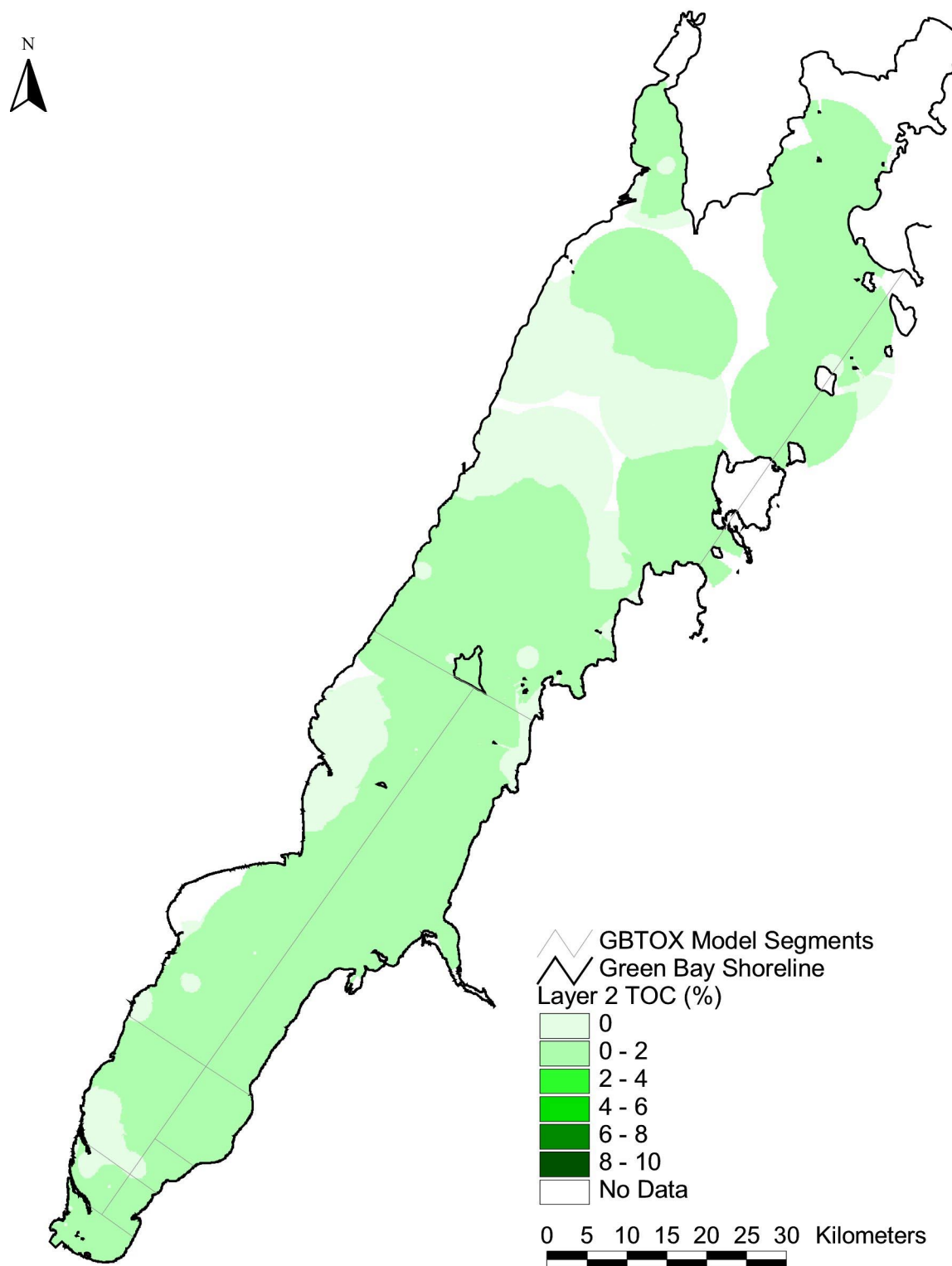


Figure 5-13. Total organic carbon (%) in Layer 2 (2-4 cm).

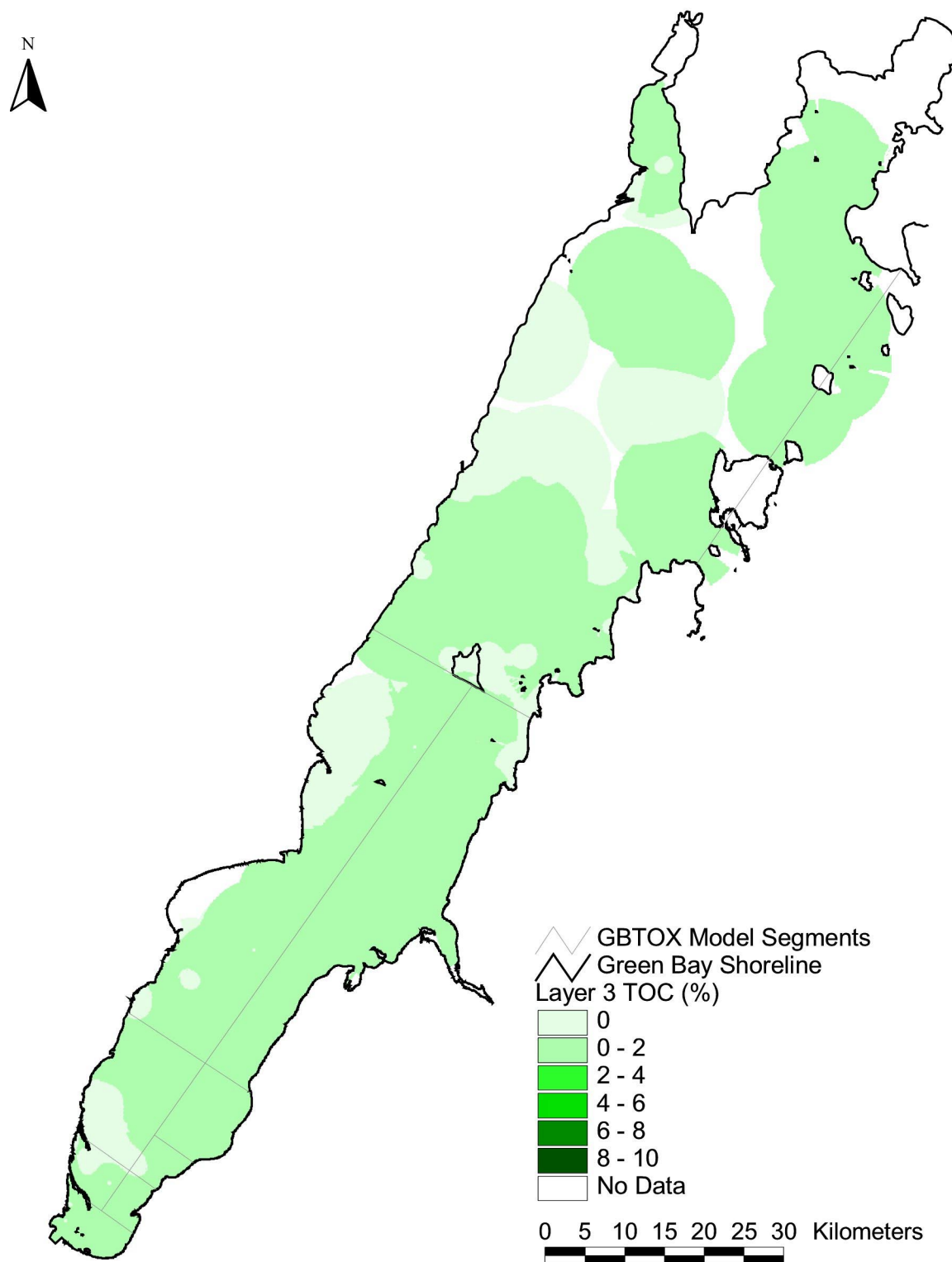


Figure 5-14. Total organic carbon (%) in Layer 3 (4-6 cm).

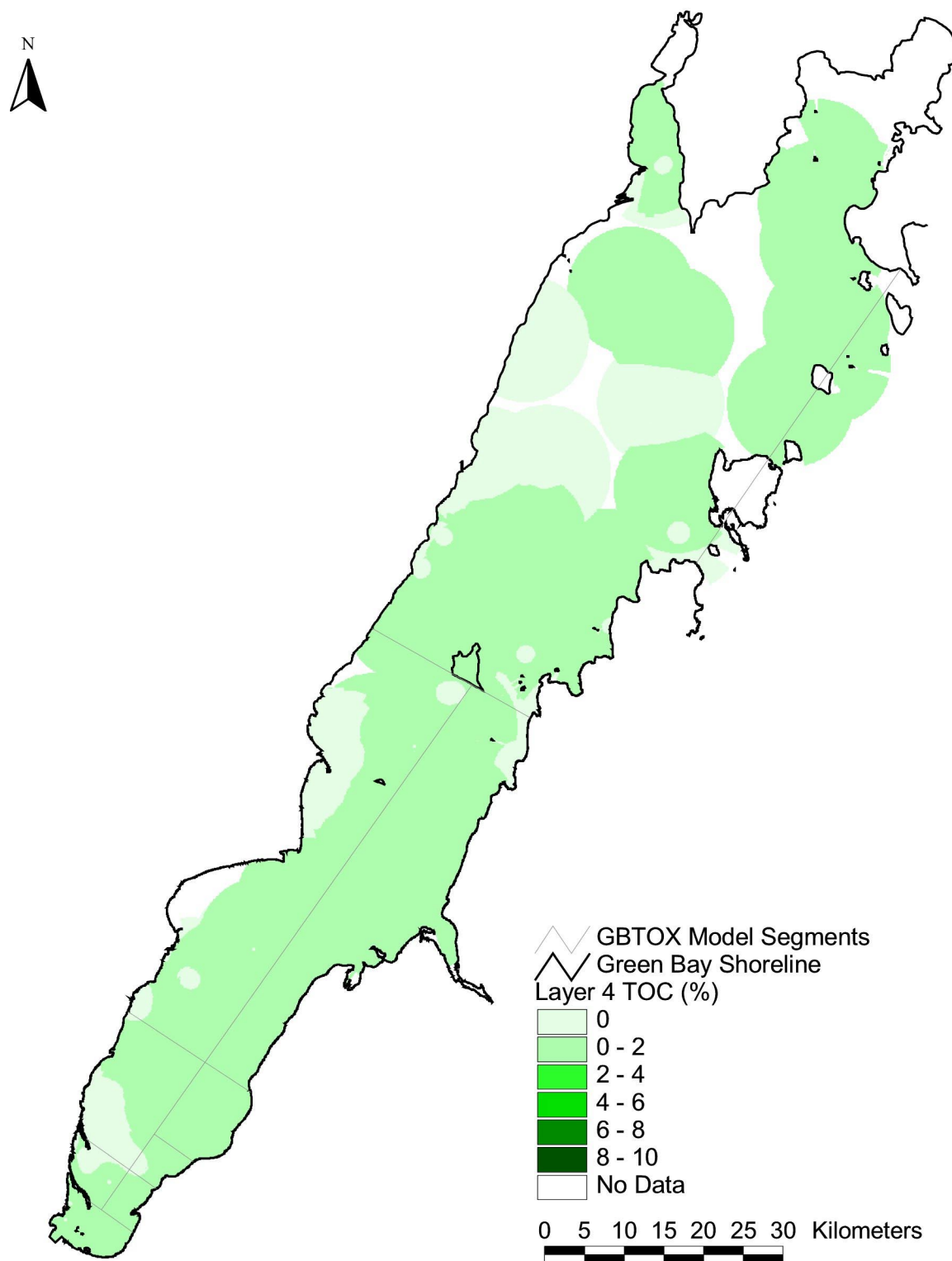


Figure 5-15 Total organic carbon (%) in Layer 4 (6-10 cm).

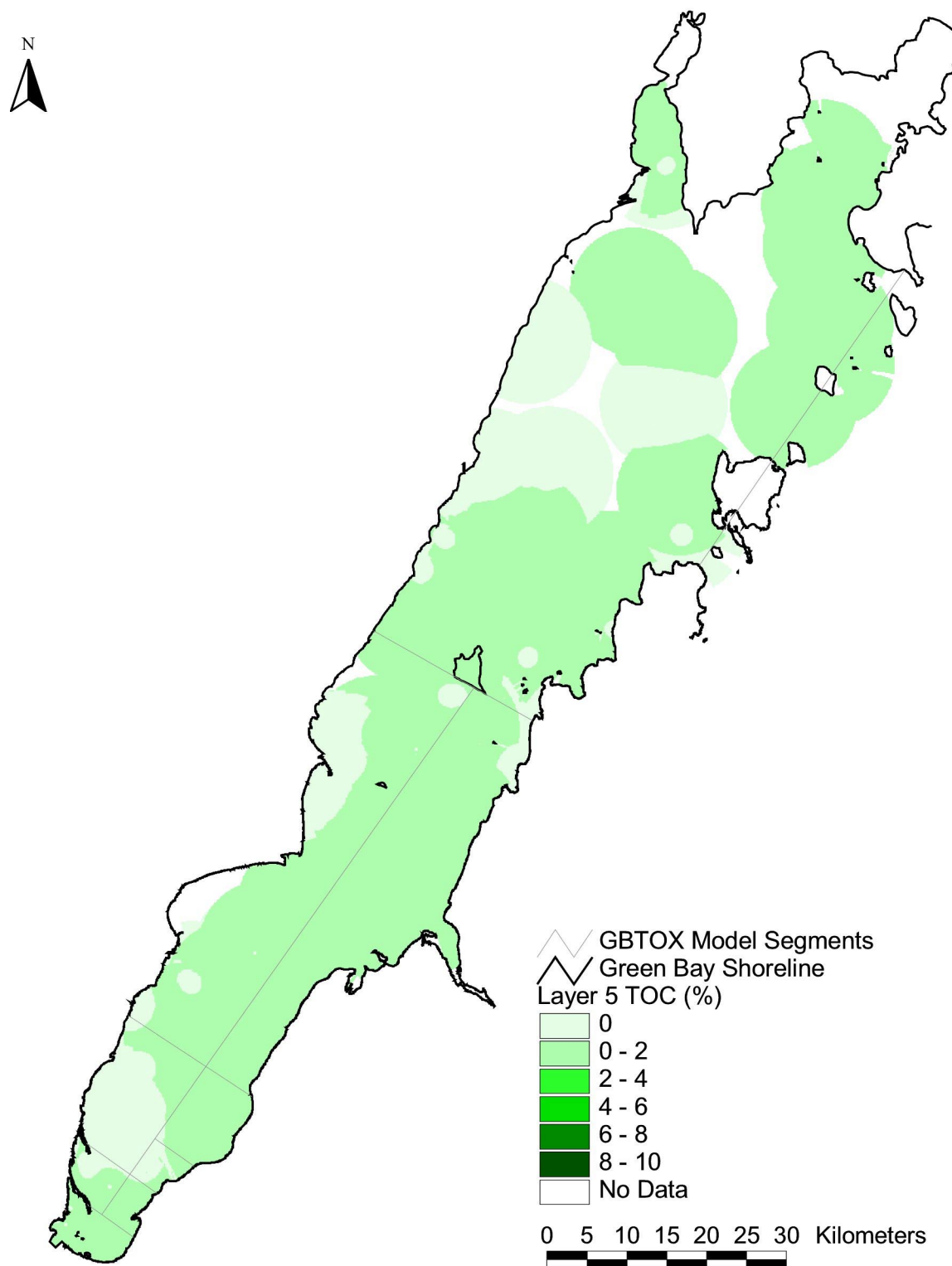


Figure 5-16. Total organic carbon (%) in Layer 5 (>10 cm).

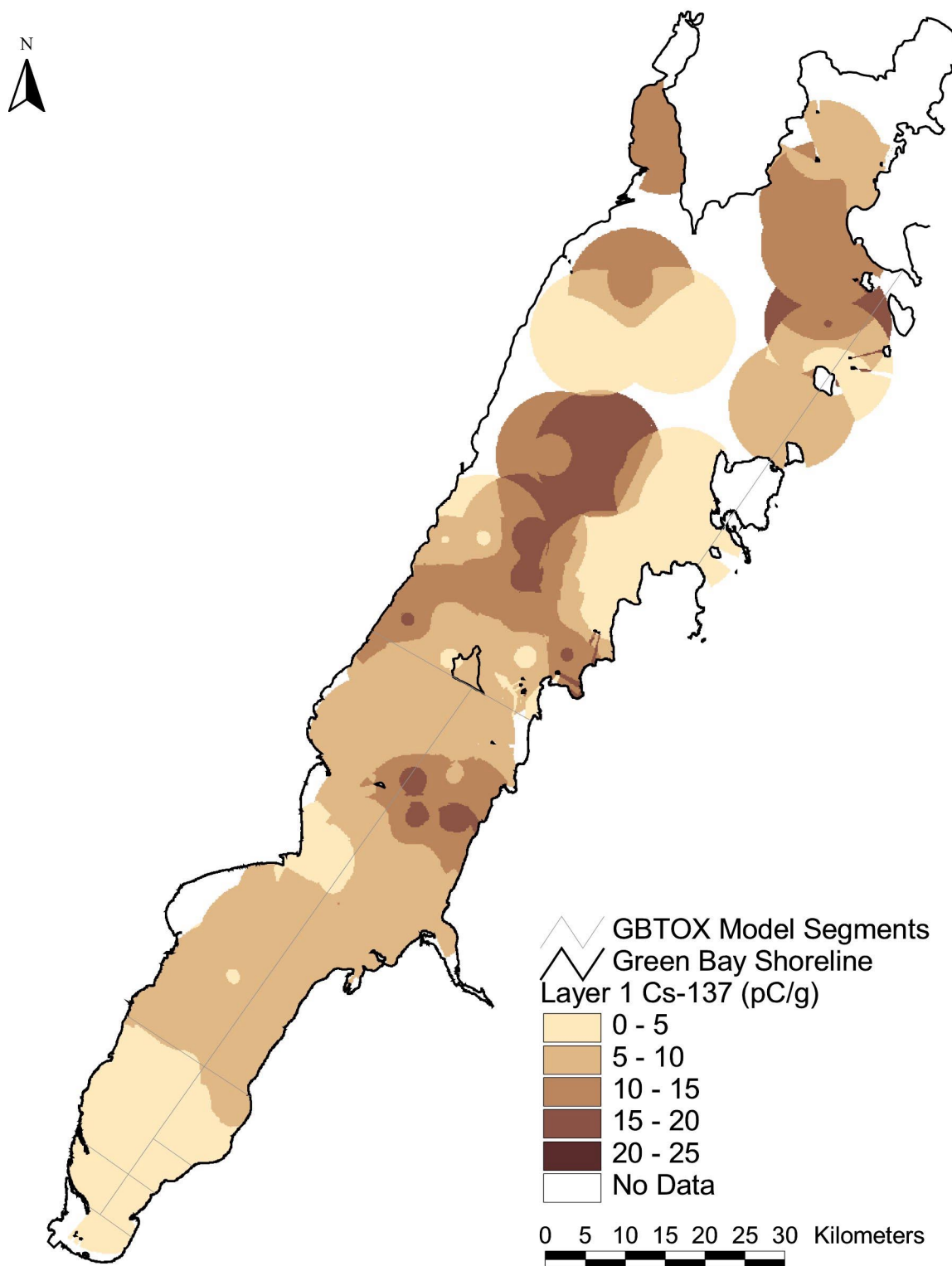


Figure 5-17. Cesium-137 (pC/g) in Layer 1 (0-2 cm).

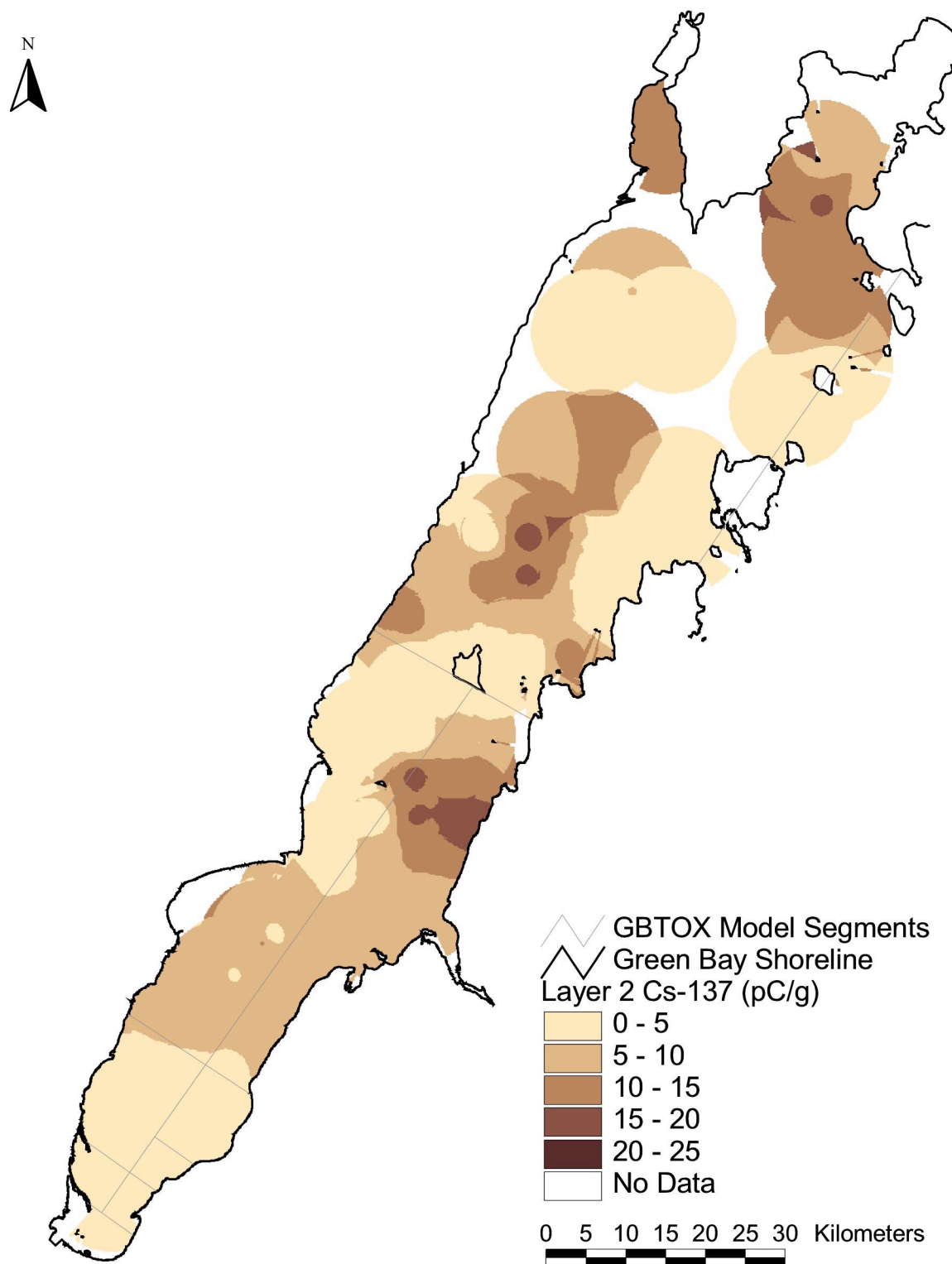


Figure 5-18. Cesium-137 (pC/g) in Layer 2 (2-4 cm).

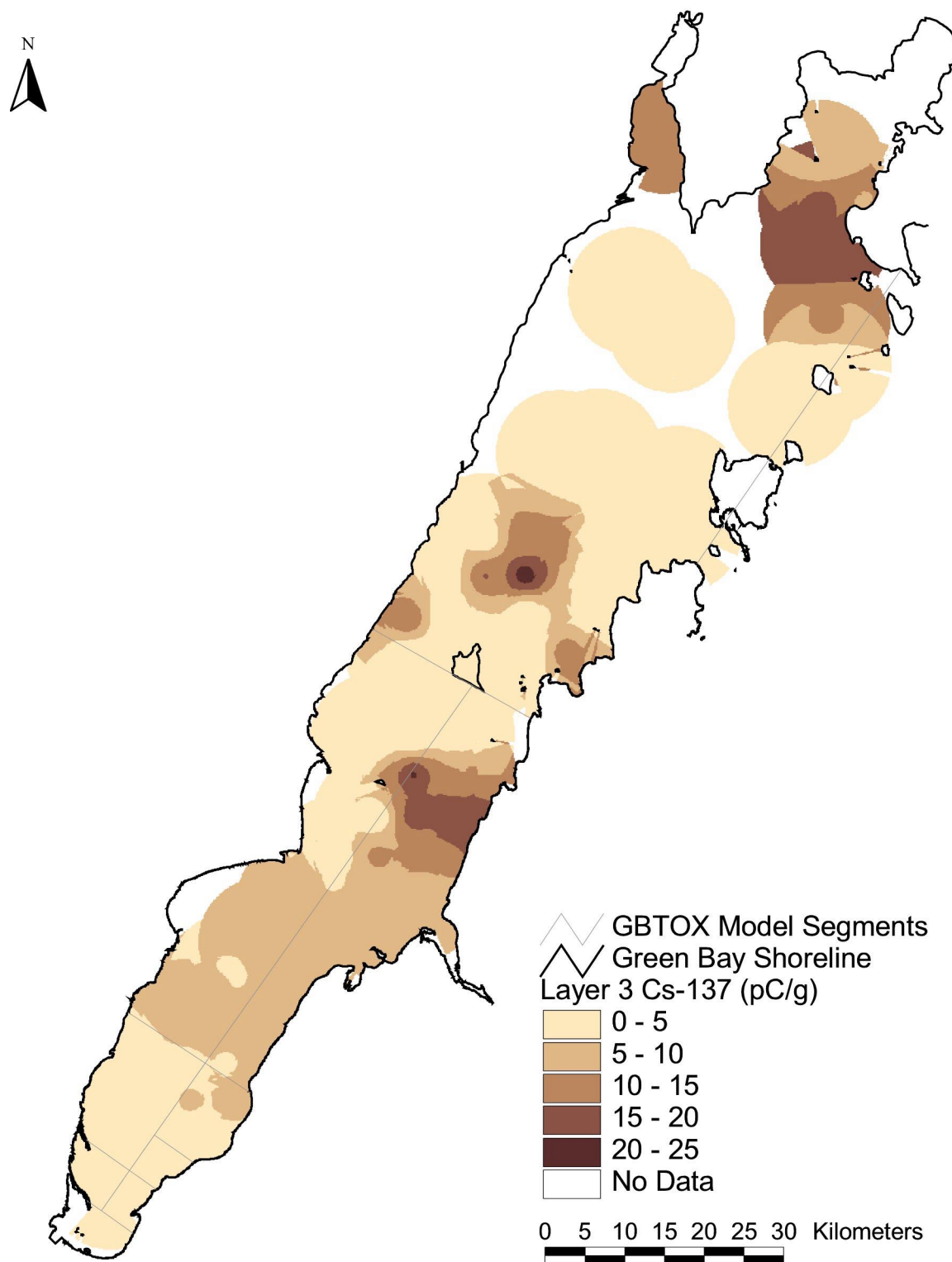


Figure 5-19. Cesium-137 (pC/g) in Layer 3 (4-6 cm).

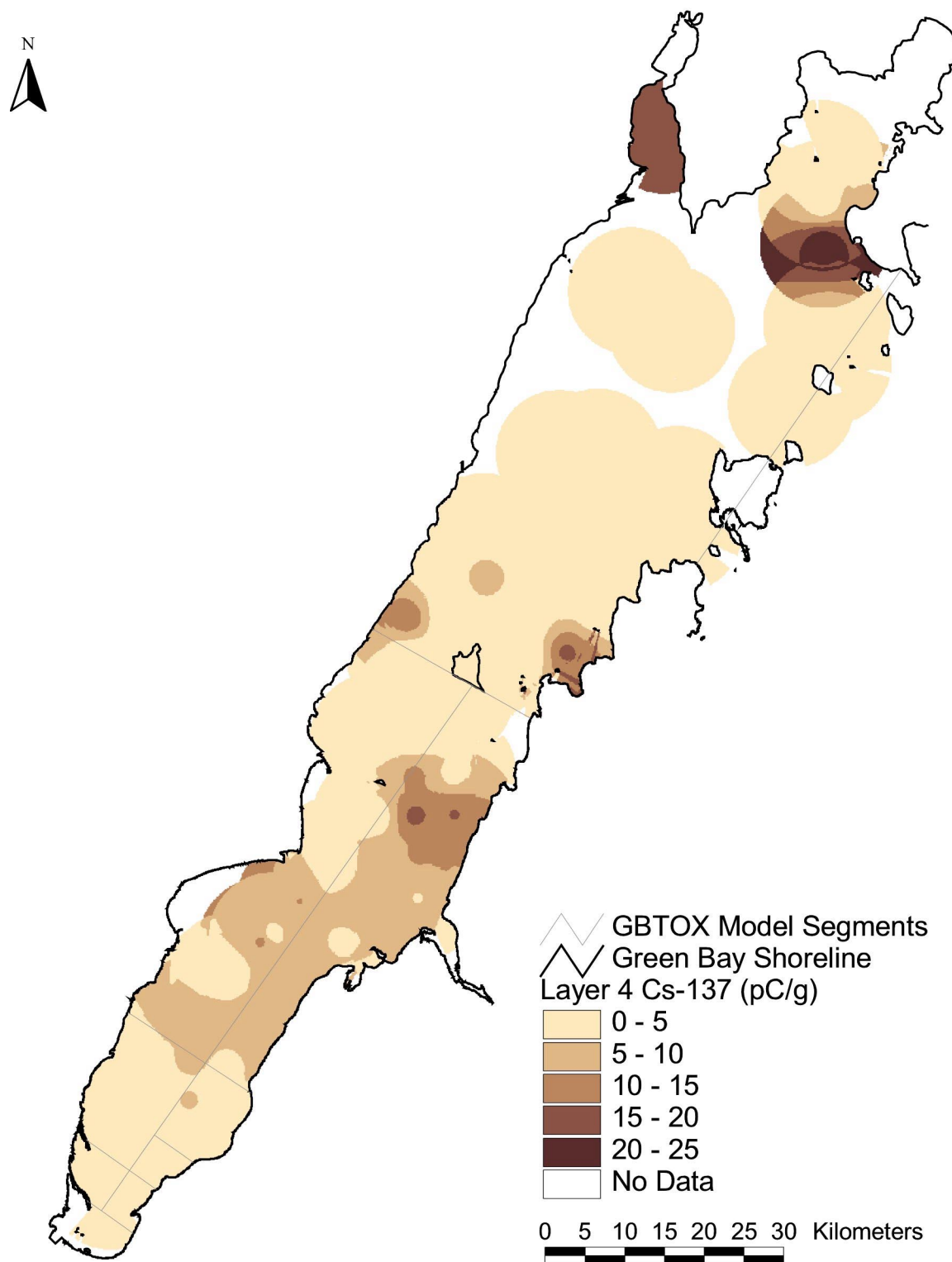


Figure 5-20. Cesium-137 (pC/g) in Layer 4 (6-10 cm).

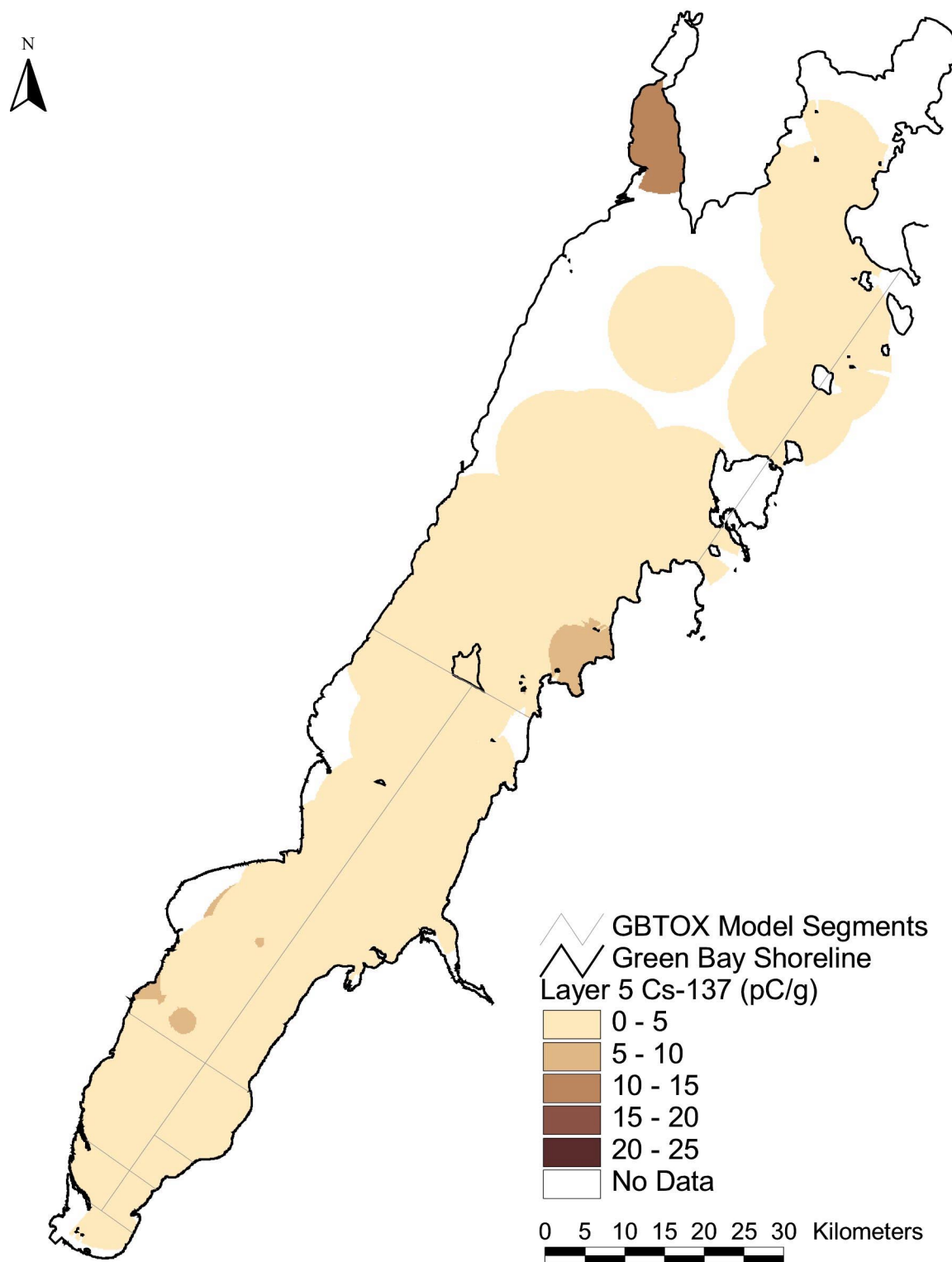


Figure 5-21. Cesium-137 (pCi/g) in Layer 5 (>10 cm).

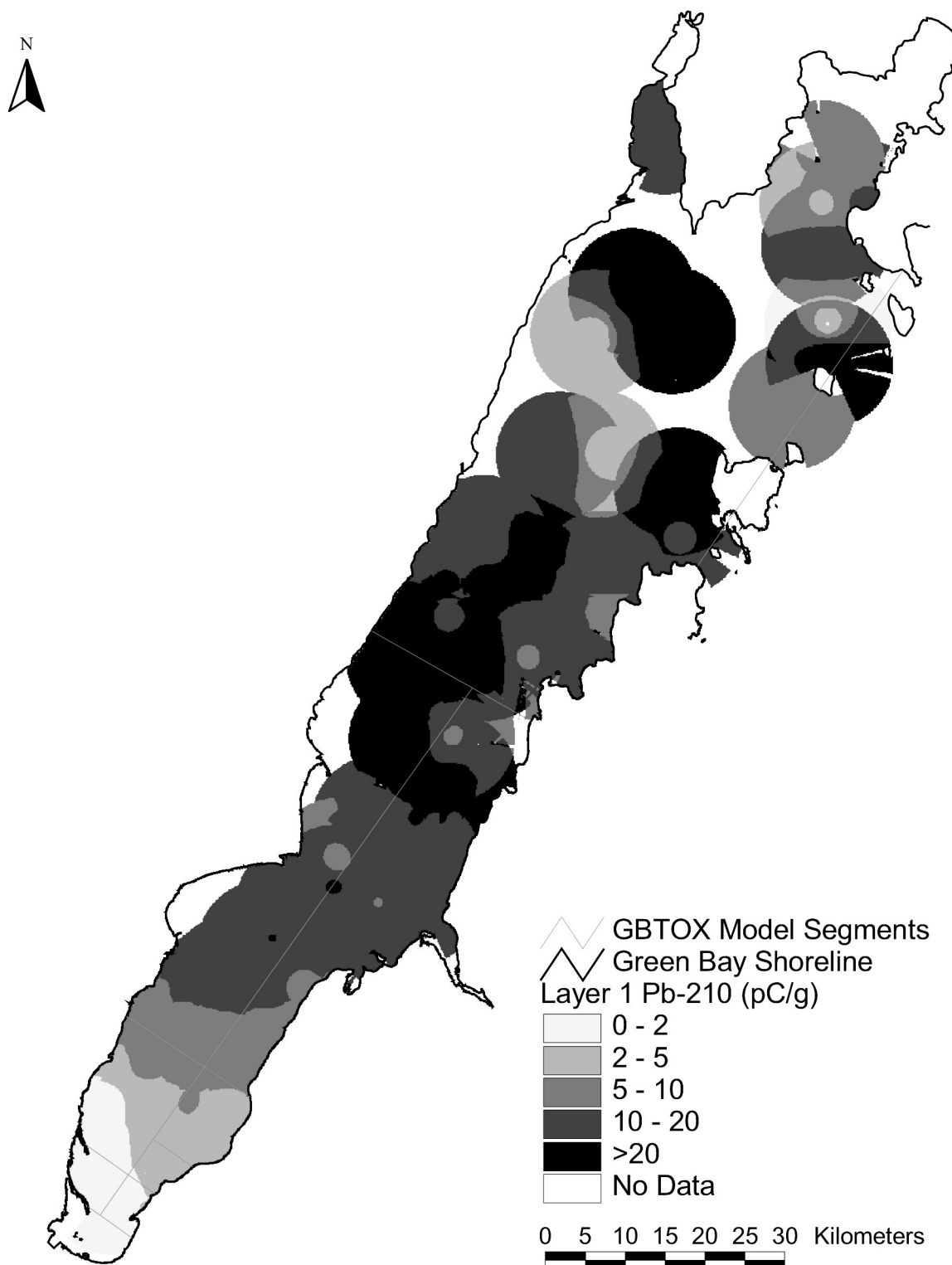


Figure 5-22. Lead-210 (pC/g) in Layer 1 (0-2 cm).

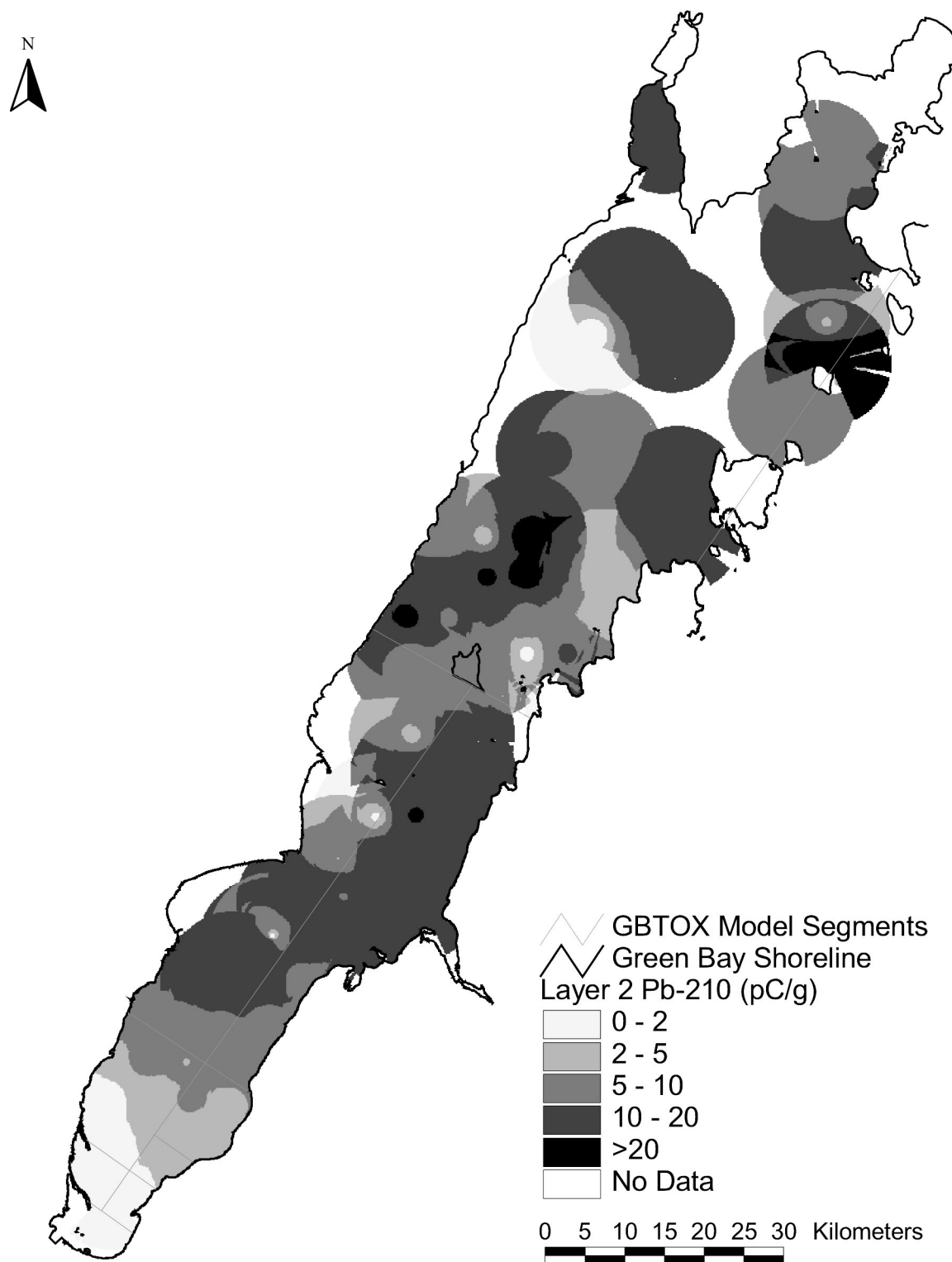


Figure 5-23. Lead-210 (pC/g) in Layer 2 (2-4 cm).

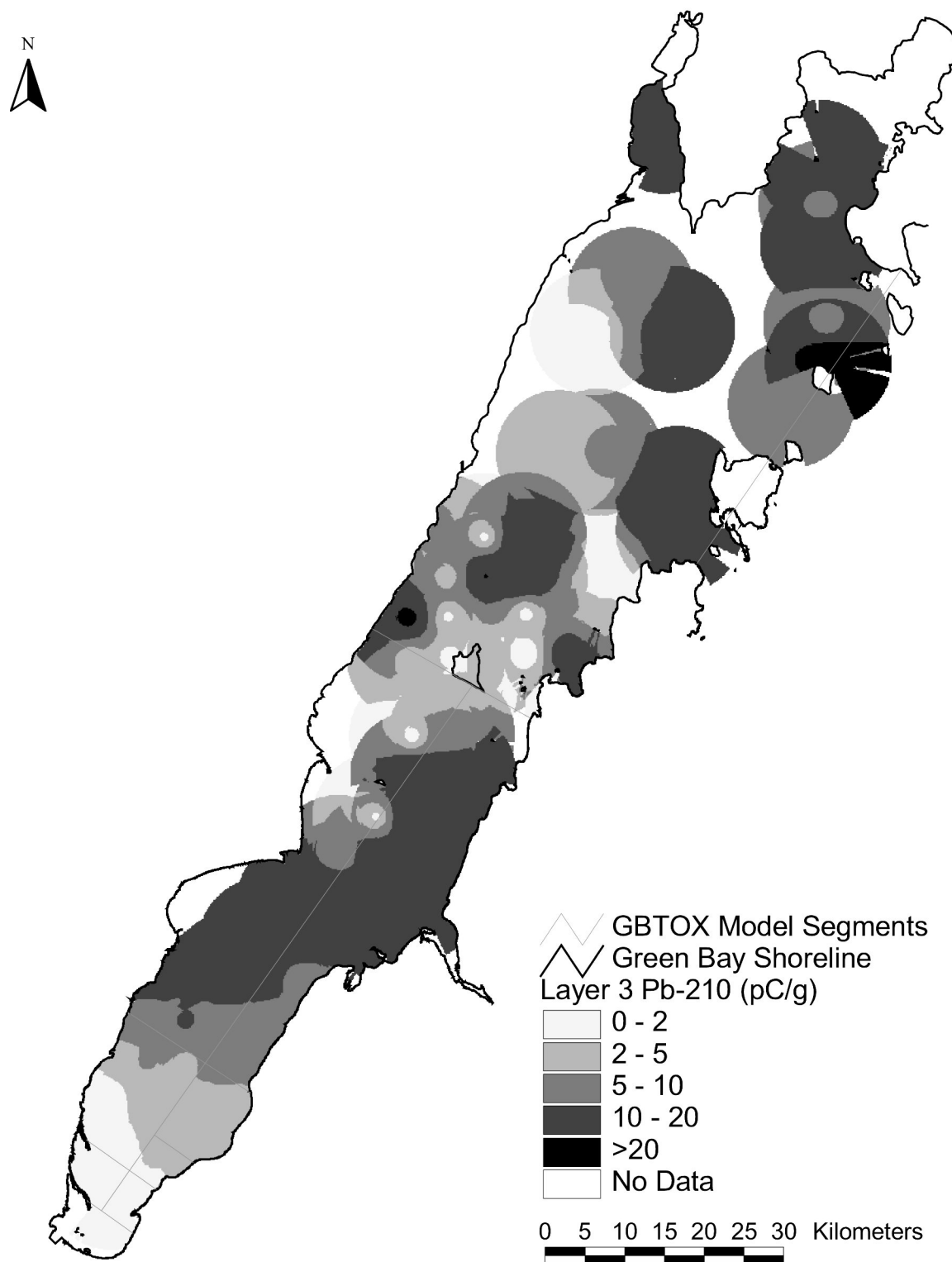


Figure 5-24. Lead-210 (pC/g) in Layer 3 (4-6 cm).

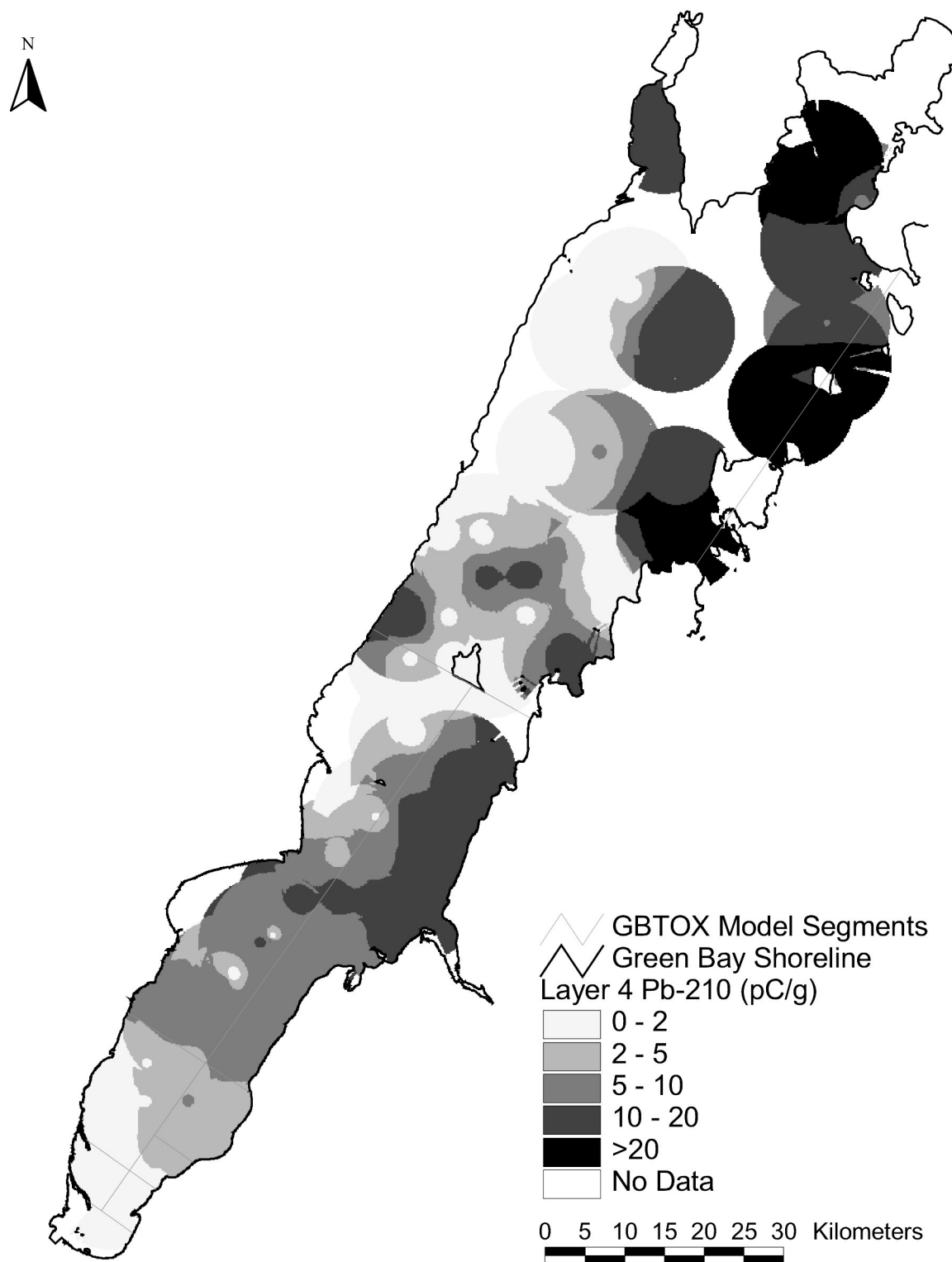


Figure 5-25. Lead-210 (pC/g) in Layer 4 (6-10 cm).

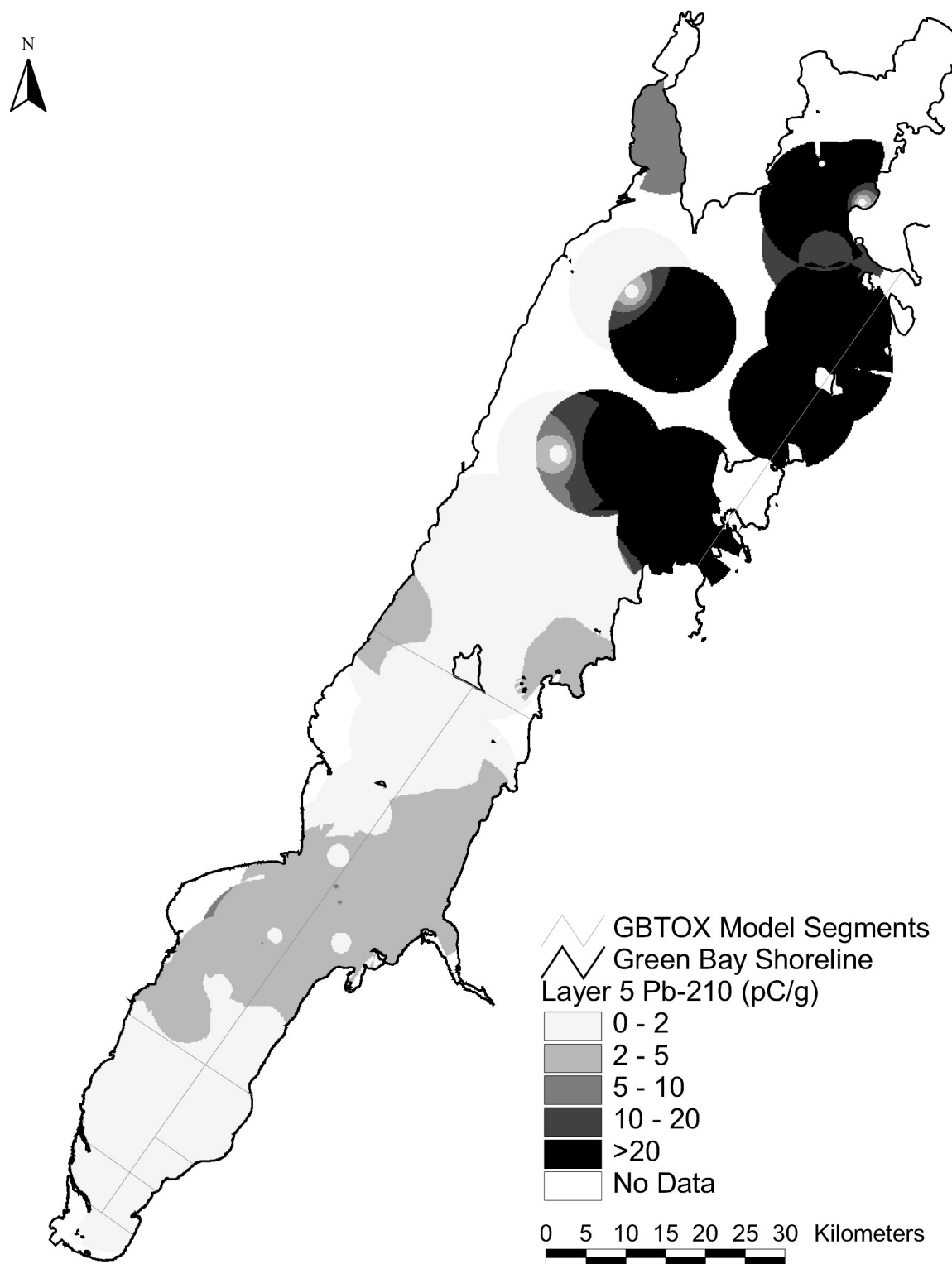


Figure 5-26. Lead-210 (pC/g) in Layer 5 (>10 cm).

5.7. PARTICLE SIZE DISTRIBUTION

Particle size distribution, measured as percent of a sample which is composed of sand, silt and clay particles, was interpolated for layer 1. For illustrative purposes, particle size distribution samples with depth and location information have been supplemented with those that do not have associated depths. These data were all assumed to be within layer 1. Particle size distribution interpolation results for layer 1 are presented in Figures 5-23 through 5-25 for sand, silt and clay, respectively.

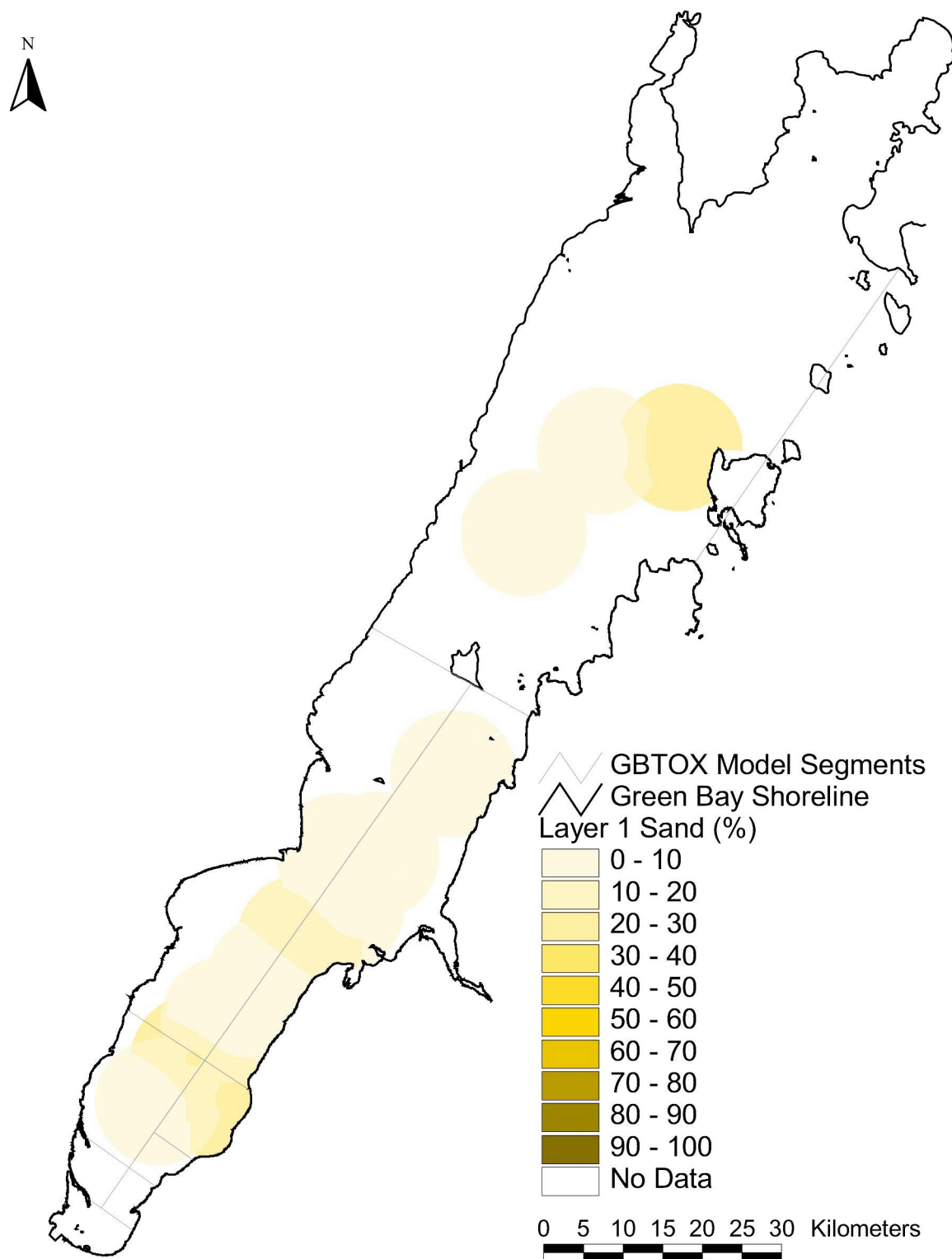


Figure 5-27. Sand fraction in Layer 1 (0-2 cm).

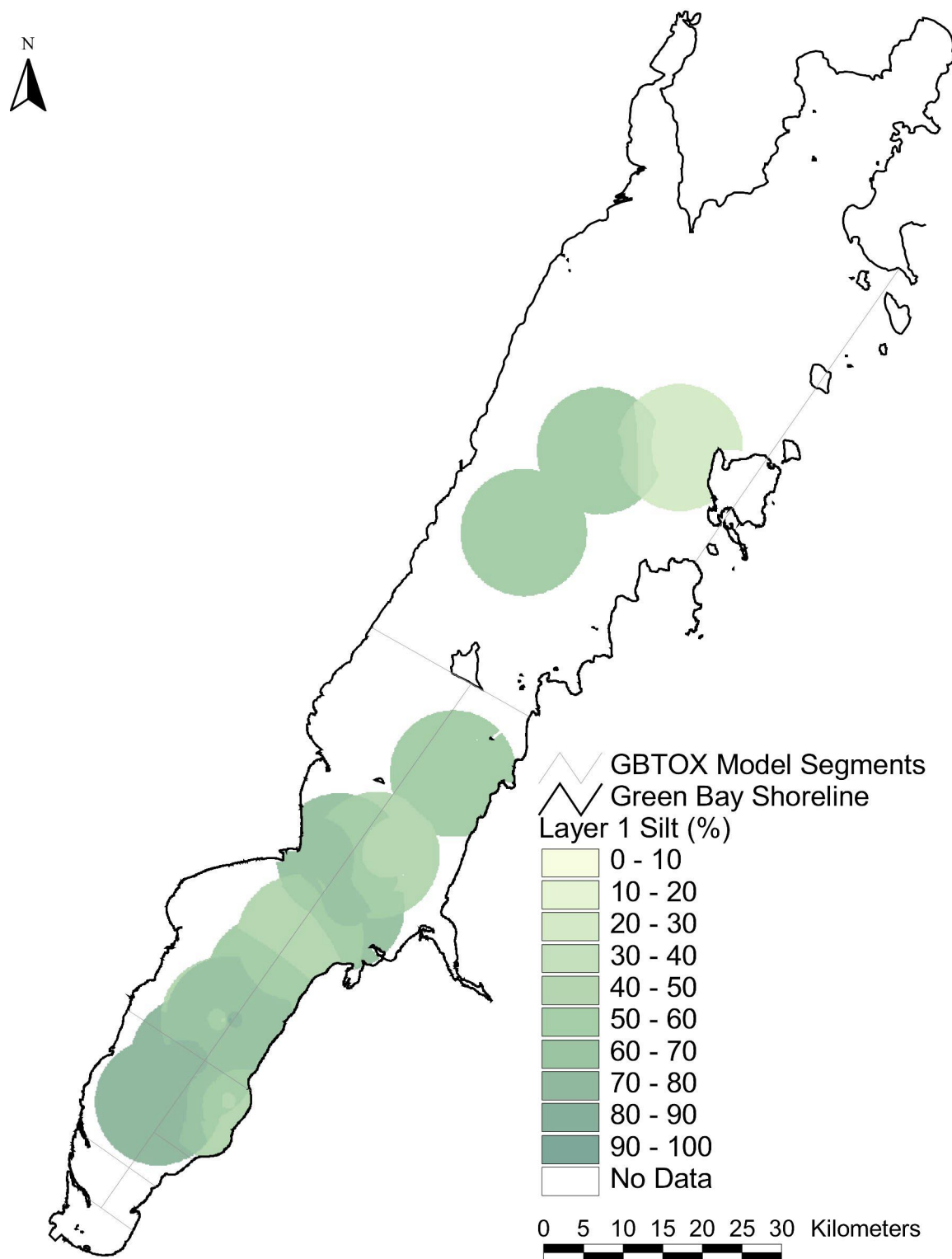


Figure 5-28. Silt fraction in Layer 1 (0-2 cm).

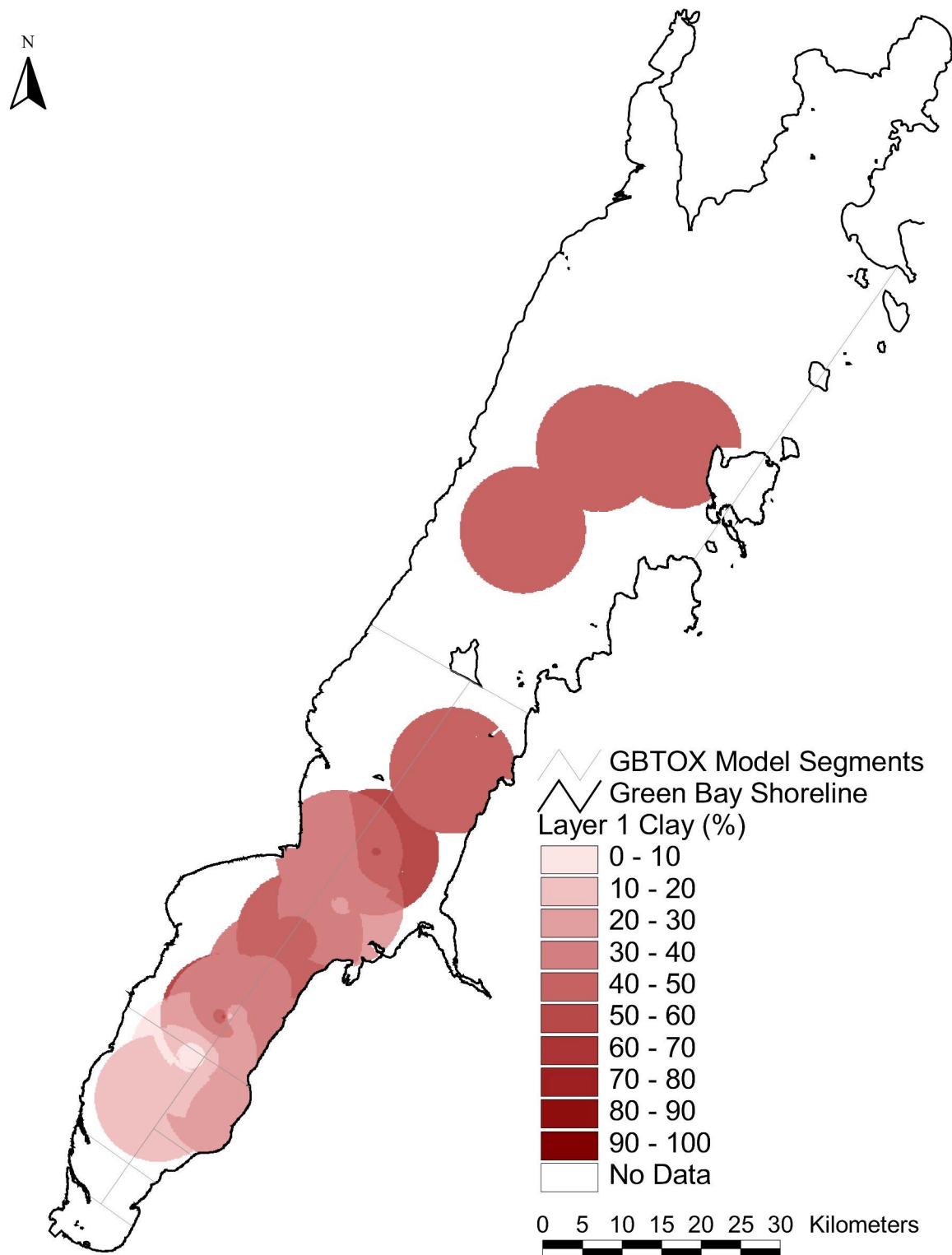


Figure 5-29. Clay fraction in Layer 1 (0-2 cm).

6.0 UNCERTAINTY

6.1. AREAL EXTENT OF SEDIMENTS

Sediment volume and chemical mass inventory estimates depend on the assumed areal (horizontal) extent of sediments in Green Bay. However, the full areal extent of sediments in Green Bay is not well defined. None of the available data sets or the sediment survey conducted by Moore et al. (1973) provided a complete description of sediment occurrence in the Bay. For example, during the GBMBS some sediment cores were collected in areas classified as gravel by Moore et al. Since sediment volume and chemical mass inventory estimates depend on estimates of surface area, underestimating the areal extent of sediments will cause volume and mass estimates to underestimate the true volume and mass in the bay. As defined by the sediment bed masks (described in Section 4.5.5), the areal extent of sediment in Green Bay was underestimated.

The “cohesive” sediment bed mask represented an attempt to merge GBMBS sediment coring locations with the sediment classifications from Moore et al. (1973). However, the areas delineated by that bed mask were limited to sediments assumed to be “cohesive.” Similarly, the areas delineated by the “soft” sediment bed mask were limited to sediments assumed to be “soft” (i.e. not sand, gravel, or hardpan, etc.) “Non-cohesive” sediments are still sediments and should be included in estimates of total sediment volume. Similarly, PCBs present in “non-cohesive” sediments are still PCBs and should be included in estimates of PCB mass inventory. Exclusion of “non-cohesive” areas introduces an underestimation bias into sediment volume and mass calculations. Although beyond the resources available to complete this bed mapping effort, a more complete approach to estimating sediment volume and chemical masses might be to delineate sediment areas as “cohesive”, “non-cohesive”, or no sediment (hardpan).

It is worth noting the “cohesive” sediment bed mask designates a large part of the surface area of the inner-most part of Green Bay as “non-cohesive” (not included). However, it is also worth noting that sediments from the inner-most part of the bay were not classified as part of the Moore et al. survey or sampled as part of GBMBS. This is significant because the excluded area contains the path of the Lower Fox River “plume”. Given the large load of cohesive sediment and associated PCBs the river transports to the bay, it is reasonable to expect that extensive cohesive sediment deposits with relatively high PCB concentrations may exist in the plume area. The “soft” sediment bed mask includes the Lower Fox River plume in the delineated area of “soft” sediment.

6.2. SEDIMENT THICKNESS (VERTICAL EXTENT OF SEDIMENTS)

Sediment volume and chemical mass inventory estimates depend on the assumed vertical extent of sediment in the bay. However, sediment thickness was not measured as part of any data collection effort for Green Bay. Depth of analysis is a surrogate for sediment thickness. Bulk density was sampled to the greatest depths in the sediment column and provided the minimum

bound for sediment thickness. However, at many sampling locations, sediments likely exist at depths greater than the depths sampled because hardpan was not encountered during sampling. Underestimating the vertical extent of sediments will cause volume and mass estimates to underestimate the true volume and mass (as long as the chemical concentration is greater than zero at that depth interval) in the bay. Since it is likely that the vertical extent of sediments were underestimated, it is possible that sediment volume and PCB mass (since PCB concentrations were typically greater than zero in the deepest core slice analyzed) were underestimated.

6.3. SPATIAL VARIABILITY OF FIELD OBSERVATIONS

Data were available for only a relatively small number of locations in the bay. Even after a considerable data search, most of the data available for interpolation were collected during the GBMBS. In general, samples from the GBMBS were collected on a 5 km by 5 km grid. This small number of data points was then used to estimate sediment bed properties over the broad area of Green Bay. However, it is reasonable to expect that sediment properties such as chemical concentrations to vary over spatial scales much smaller than the 5 km by 5 km sample collection grid, especially near regions of chemical influx such as the Lower Fox River mouth. Particularly for PCBs, it is reasonable to expect that chemical concentrations near the river mouth would be greater than concentrations further out into the bay. Unfortunately, large portions of the innermost part of Green Bay were never sampled, especially the area associated with the Lower Fox River plume. However, PCB concentrations at those few locations that were sampled averaged more than 5 mg/kg with a maximum of 24 mg/kg. In contrast, PCB concentrations at all other locations averaged only 0.32 mg/kg with a maximum of less than 2 mg/kg. Clearly, this order of magnitude variation in PCB concentrations suggests that the full spatial variability of PCB concentrations is not well characterized. PCB concentrations and mass inventory estimates are very likely underestimated. This conclusion may also hold for other sediment bed properties as well. Therefore, these interpolations are best viewed as broad estimates of bay conditions.

The spatial variability of bulk density observations is worth noting when considering PCB mass inventory estimates. PCB concentrations are expressed as a mass of PCB per mass of sediment. Bulk density expresses the mass of sediment per volume. Since computation of PCB mass is a function of concentration, bulk density, surface area, and thickness, the results of the bulk density interpolations directly affect the PCB mass estimate. Therefore, the uncertainty associated with the PCB mass inventory estimate was also influenced by the highly variable nature of the bulk density observations. For example, the vertical average bulk density of GBMBS samples was 0.30 g/cm³ while the average density of the 0 to 1 cm slice was 0.18 g/cm³. In contrast, the vertical average of samples from the WDNR and BBL data sets was 0.51 gm/cm³ while the average density of the 0 to 10 cm slice was 0.77 g/cm³. It was not possible to determine whether these differences in bulk density observations were the result of true spatial variability in sediment densities or the result of differences in sample collection and analysis protocols between the various studies.

It should again be recognized that the sediment volume and PCB mass inventory estimates may represent a lower bound or minimum (Min) value. Ideally, it would be desirable to compute a range of values to more fully bound these estimates. If reliable information regarding the

absolute total thickness of sediments, sampling device penetration and sample recovery were available, it would be possible to develop “middle” (Mid) or maximum (Max) volume and mass estimates according to the procedures described in Technical Memorandum 2e (WDNR, 1999). Unfortunately, at most locations this information was not reported and could not be otherwise approximated. As a consequence, it was not possible to meaningfully estimate Mid or Max estimates of sediment volume and PCB mass for Green Bay.

6.4. TEMPORAL VARIABILITY OF FIELD OBSERVATIONS

The large majority of observations used in these interpolations are from cores collected during the GBMBS. Samples for that study were collected between 1986 and 1991 with most PCB samples being collected in the 1988 to 1991 period. Since the majority of the observations were collected during a relatively narrow time frame, the interpolation results are most representative of the conditions that existed around 1989-90.

Some data were obtained for periods outside the GBMBS time frame. These data were included in interpolations when sufficient locational information was available. However, the scarcity of data from outside the GBMBS period prevents even a sketchy estimation of sediment bed properties throughout the bay for other time periods.

6.5. IDW WEIGHTING EXPONENT AND RADIUS OF INFLUENCE

The IDW interpolation approach assumes that neighboring data points can reliably tell us information in order to estimate sediment parameters. The 8,000-meter radius of the IDW tool defines the “neighborhood” of data points. It is recognized that significant variation in environmental variables occurs on a much smaller spatial scale than 8,000 meters. The jackknife approach used to select the radius of influence helps minimize but does not eliminate the uncertainty associated with the spatial variability among data points.

The jackknifing results (see Appendix A) suggested that the $r = 8,000$, $n = 2$ combination was an “optimal” choice for predicting known values of total PCBs in consideration of the objectives to maximize coverage, minimize error, and use consistent IDW parameters for all interpolations. The radius of 8,000, which minimized error for PCBs, was somewhat larger than the optimal radii identified for TOC and bulk density, and the use of a consistent radius for all variables is a potential source of error for these interpolations. Based on the jackknifing results for $r = 8,000$, $n = 2$, the estimated average absolute residual errors are 154 ug/kg for PCBs, 0.24 g/cm³ for bulk density, and 1.7% for TOC. These prediction errors for known data points provide the best available estimate of interpolation errors for locations where data do not exist.

However, it is worth noting that the goal of minimum interpolation error was effectively given greater weight than the goal of maximizing areal coverage. The minimum possible prediction error was achieved at the expense of yielding interpolations that cover 100% of the bay surface area. Failure to achieve 100% areal coverage introduces an underestimation bias into sediment volume and PCB mass estimates. The areal coverage bias could be eliminated by selection of a larger radius (to cover 100% of the area) and a greater exponent value to minimize interpolation

error for that radius. As shown in Figure 4-15 and Table 4-2, 100% areal coverage could be achieved by selecting a radius value on the order of 15,000 m. In Section 4.5.4, it was also noted that larger exponent values tended to produce lower prediction error when the radius is set at values greater than about 10,000 m. As shown in Figure 4-12, prediction error when $r > 10,000$ m is lower when $n > 2$. Although beyond the resources available to complete this effort, a more complete approach to estimating sediment volume and chemical masses would have been to include Lower Fox River plume and other areas of the inner bay as “cohesive” sediment and selecting larger r and n values such as $r = 15,000$ m and $n = 5$.

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APPENDIX A

Table A-1. Jackknifing results: total PCB concentration.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	185.209	0.399	247.609	11.547
5,000	3	186.806	0.402	249.460	9.027
5,000	4	187.759	0.404	250.630	7.842
5,000	5	188.327	0.406	251.230	7.331
6,000	2	176.705	0.381	231.741	4.826
6,000	3	177.256	0.382	232.547	1.950
6,000	4	178.427	0.384	233.671	0.466
6,000	5	179.194	0.386	234.320	-0.187
7,000	1	168.191	0.362	227.357	9.874
7,000	2	164.233	0.354	222.543	7.496
7,000	3	165.264	0.356	223.504	4.656
7,000	4	166.812	0.359	225.058	3.034
7,000	5	168.263	0.362	226.271	2.186
7,500	2	153.989	0.332	208.929	10.337
7,500	3	156.931	0.338	211.980	6.908
7,500	4	160.377	0.345	215.548	4.777
7,500	5	163.307	0.352	218.625	3.510
8,000	1	160.463	.346	213.728	14.472
8,000	2	154.418	0.333	208.857	10.802
8,000	3	157.190	0.339	211.801	7.225
8,000	4	160.536	0.346	215.387	4.988
8,000	5	163.406	0.352	218.503	3.646
9,000	1	162.644	0.350	218.550	-4.321
10,000	1	169.876	0.366	230.527	16.823
10,000	2	158.688	0.342	216.956	12.659
10,000	3	159.139	0.343	215.542	8.699
10,000	4	160.919	0.347	216.710	6.161
10,000	5	162.677	0.350	218.491	4.547

Table A-1 (continued). Jackknifing results: total PCB concentration.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
15,000	1	171.956	0.370	236.446	22.515
15,000	2	158.643	0.342	219.304	19.086
15,000	3	156.570	0.337	214.731	13.453
15,000	4	157.482	0.339	214.291	9.212
15,000	5	158.936	0.342	215.510	6.471
20,000	1	178.359	0.384	243.511	27.604
20,000	2	161.935	0.349	222.876	21.726
20,000	3	158.169	0.341	216.093	14.899
20,000	4	158.140	0.341	214.726	9.973
20,000	5	159.292	0.343	215.650	6.878

Table A-2. Jackknifing results: dry bulk density.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	0.202	0.593	0.373	-0.0039
5,000	3	0.205	0.599	0.377	-0.0025
5,000	4	0.206	0.604	0.381	-0.0009
5,000	5	0.207	0.608	0.383	0.0004
6,000	2	0.197	0.577	0.361	0.0017
6,000	3	0.198	0.581	0.364	0.0028
6,000	4	0.199	0.584	0.367	0.0037
6,000	5	0.200	0.586	0.369	0.0044
7,000	2	0.226	0.661	0.396	-0.0195
7,000	3	0.228	0.668	0.399	-0.0189
7,000	4	0.230	0.673	0.401	-0.0184
7,000	5	0.231	0.676	0.404	-0.0182
7,500	2	0.237	0.694	0.418	-0.0047
7,500	3	0.239	0.702	0.422	-0.0042
7,500	4	0.241	0.707	0.424	-0.0038
7,500	5	0.242	0.710	0.427	-0.0037
8,000	2	0.238	0.697	0.419	-0.0046
8,000	3	0.240	0.703	0.422	-0.0041
8,000	4	0.242	0.708	0.425	-0.0038
8,000	5	0.242	0.711	0.427	-0.0037

Table A-3. Jackknifing results: total organic carbon.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	1.609	0.314	2.373	-0.1717
5,000	3	1.615	0.315	2.378	-0.1757
5,000	4	1.617	0.316	2.380	-0.1776
5,000	5	1.618	0.316	2.381	-0.1787
6,000	2	1.412	0.276	2.098	-0.0814
6,000	3	1.421	0.278	2.107	-0.0866
6,000	4	1.425	0.278	2.112	-0.0899
6,000	5	1.428	0.279	2.115	-0.0923
7,000	2	1.581	0.309	2.404	0.1154
7,000	3	1.591	0.311	2.408	0.0880
7,000	4	1.595	0.312	2.412	0.0658
7,000	5	1.603	0.313	2.416	0.0481
7,500	1	1.636	0.319	2.385	0.0325
7,500	2	1.638	0.320	2.390	0.0181
7,500	3	1.635	0.319	2.399	0.0010
7,500	4	1.629	0.318	2.409	-0.0132
7,500	5	1.632	0.319	2.418	-0.0245
8,000	2	1.739	0.340	2.588	-0.1037
8,000	3	1.735	0.339	2.596	-0.1205
8,000	4	1.729	0.338	2.604	-0.1347
8,000	5	1.732	0.338	2.613	-0.1461

Table A-4. Jackknifing results: depth of analysis of total PCBs.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	0.0412	0.328	0.0620	-0.0045
5,000	3	0.0419	0.333	0.0632	-0.0042
5,000	4	0.0421	0.334	0.0636	-0.0039
5,000	5	0.0421	0.334	0.0638	-0.0038
6,000	2	0.0419	0.333	0.0619	-0.0058
6,000	3	0.0426	0.339	0.0633	-0.0057
6,000	4	0.0427	0.340	0.0638	-0.0055
6,000	5	0.0427	0.339	0.0639	-0.0053
7,000	2	0.0434	0.345	0.0674	-0.0011
7,000	3	0.0444	0.353	0.0689	-0.0012
7,000	4	0.0448	0.356	0.0695	-0.0011
7,000	5	0.0449	0.357	0.0698	-0.0010
7,500	2	0.0441	0.351	0.0675	-0.0008
7,500	3	0.0449	0.357	0.0690	-0.0010
7,500	4	0.0451	0.359	0.0696	-0.0010
7,500	5	0.0452	0.359	0.0699	-0.0010
8,000	2	0.0441	0.350	0.0675	-0.0008
8,000	3	0.0449	0.357	0.0690	-0.0010
8,000	4	0.0451	0.359	0.0696	-0.0010
8,000	5	0.0452	0.359	0.0699	-0.0010

Table A-5. Jackknifing results: depth of analysis for bulk density.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	0.1522	0.455	0.2051	-0.0025
5,000	3	0.1557	0.466	0.2116	-0.0053
5,000	4	0.1586	0.474	0.2166	-0.0084
5,000	5	0.1606	0.480	0.2206	-0.0115
6,000	2	0.1494	0.447	0.2008	0.0055
6,000	3	0.1532	0.458	0.2072	0.0027
6,000	4	0.1563	0.467	0.2123	-0.0006
6,000	5	0.1585	0.474	0.2165	-0.0039
7,000	2	0.1529	0.457	0.2026	0.0096
7,000	3	0.1567	0.469	0.2090	0.0076
7,000	4	0.1596	0.477	0.2140	0.0049
7,000	5	0.1616	0.483	0.2182	0.0021
7,500	2	0.1452	0.434	0.1944	0.0087
7,500	3	0.1499	0.448	0.2016	0.0064
7,500	4	0.1538	0.460	0.2076	0.0035
7,500	5	0.1566	0.468	0.2127	0.0006
8,000	2	0.1459	0.436	0.1952	0.0083
8,000	3	0.1502	0.449	0.2020	0.0060
8,000	4	0.1540	0.461	0.2079	0.0032
8,000	5	0.1568	0.469	0.2129	0.0003

Table A-6. Jackknifing results: depth of analysis for TOC.

Radius (m)	Weighting exponent	Average absolute residual	Normalized residual index	Square root of average of squared residuals (RMS)	Average signed residual
5,000	2	0.0340	0.209	0.0519	0.0019
5,000	3	0.0343	0.211	0.0523	0.0022
5,000	4	0.0344	0.212	0.0525	0.0024
5,000	5	0.0345	0.212	0.0526	0.0025
6,000	2	0.0342	0.211	0.0516	0.0026
6,000	3	0.0344	0.212	0.0518	0.0030
6,000	4	0.0345	0.212	0.0520	0.0032
6,000	5	0.0345	0.212	0.0521	0.0033
7,000	2	0.0346	0.213	0.0507	0.0046
7,000	3	0.0342	0.211	0.0507	0.0045
7,000	4	0.0338	0.208	0.0507	0.0044
7,000	5	0.0335	0.207	0.0507	0.0043
7,500	2	0.0309	0.190	0.0471	0.0019
7,500	3	0.0312	0.192	0.0477	0.0024
7,500	4	0.0314	0.193	0.0482	0.0027
7,500	5	0.0316	0.194	0.0487	0.0030
8,000	2	0.0303	0.187	0.0468	0.0020
8,000	3	0.0307	0.189	0.0473	0.0025
8,000	4	0.0308	0.190	0.0479	0.0028
8,000	5	0.0311	0.191	0.0483	0.0030

APPENDIX B

Table B-1. Estimated average depth of analysis (m) for “cohesive” sediment areas of GBTOX model segments.¹

GBTOX Model Segment	Depth of Analysis (Minimum Sediment Thickness) (m)
1	0.1399
2	0.1143
3	0.1311
4	0.0978
5	0.1055
6	0.1101
7	0.1338
8	0.1488
9	0.0792

Table B-2. Estimated average dry bulk density (g/cm³) for “soft” sediment areas of GBTOX model segments.

Dry Bulk Density (g/cm ³)									
GBTOX segment									
Layer	1	2	3	4	5	6	7	8	9
0-2 cm	0.6319	0.6655	0.5075	0.6921	0.6315	0.2683	0.5559	0.1728	0.3843
2-4 cm	0.6321	0.6851	0.5118	0.7261	0.6570	0.3313	0.6661	0.2075	0.5360
4-6 cm	0.6325	0.6980	0.5168	0.7596	0.6746	0.3560	0.6544	0.2193	0.5788
6-10 cm	0.6327	0.7127	0.5206	0.8272	0.6904	0.3943	0.6828	0.2571	0.5571
> 10 cm	0.5578	0.7740	0.5069	0.9156	0.7379	0.6857	0.7051	0.3200	0.5892

¹ Depth of analysis summary based on results prepared by Limno-Tech, Inc. on behalf of the Fox River Group (thickminr80).

Table B-3. Estimated average total PCB concentration (ug/kg) for “soft” sediment areas of GBTOX model segments.

Total PCB concentration (ug/kg)									
GBTOX segment									
Layer	1	2	3	4	5	6	7	8	9
0-2 cm	2010	273	674	274	609	776	350	531	92
2-4 cm	2008	241	627	234	459	725	308	552	59
4-6 cm	2011	295	683	249	491	672	291	508	53
6-10 cm	2009	264	619	202	273	374	247	391	38
> 10 cm	2311	126	439	100	291	258	119	140	10

Table B-4. Estimated mass of total PCBs by layer for “soft” sediment areas of GBTOX model segments.²

PCB Mass (kg)										
GBTOX segment										
Layer	1	2	3	4	5	6	7	8	9	Total
0-2 cm	1,066	170	235	613	283	382	1,327	850	390	5,316
2-4 cm	1,067	157	218	496	175	341	1,031	930	286	4,701
4-6 cm	1,067	157	218	496	175	341	1,031	930	286	4,701
6-10 cm	2,134	314	436	992	350	682	2,062	1,860	572	9,402
> 10 cm	18,575	2,225	4,010	2,760	1,475	2,700	8,420	5,250	420	45,835
Total	23,909	3,023	5,117	5,357	2,458	4,446	13,871	9,820	1,954	69,955

² PCB mass inventory based on estimates prepared by Thermo-Retec, Inc. on behalf of WDNR with data as aggregated for Lower Fox River/Green Bay Remedial Investigation/Feasibility Study efforts.

Table B-5. Estimated mass of total PCBs for “soft” sediment areas of GBTOX model segments.³

GBTOX segment	Impacted Area (km ²)	PCB Contaminated Sediment Volume (m ³)	PCB inventory (kg)	PCB inventory (%)
1	41	18,580,000	23,909	34.18
2	38	12,094,000	3,023	4.32
3	24	8,908,000	5,117	7.31
4	162	46,783,000	5,357	7.66
5	26	7,932,000	2,458	3.51
6	85	25,560,000	4,446	6.36
7	500	166,069,000	13,871	19.83
8	529	189,902,000	9,820	14.04
9	702	146,525,000	1,954	2.79
Total	2,107	622,353,000	69,955	100

Table B-6. Estimated average total organic carbon (%) for “soft” sediment areas of GBTOX model segments.

TOC percentage									
GBTOX segment									
Layer	1	2	3	4	5	6	7	8	9
0-2 cm	3.55	1.50	2.31	2.24	1.94	4.02	4.00	6.46	4.35
2-4 cm	3.55	1.47	2.28	2.16	1.84	3.91	3.43	6.08	3.41
4-6 cm	3.54	1.40	2.20	1.89	1.65	3.58	3.32	5.78	3.11
6-10 cm	3.54	1.39	2.20	1.58	1.55	3.33	3.21	5.49	2.96
> 10 cm	3.54	1.39	2.16	0.91	0.95	2.10	2.78	4.82	2.56

³ Sediment volume and PCB mass inventory based on estimates prepared by Thermo-Retec, Inc. on behalf of WDNR with data as aggregated for Lower Fox River/Green Bay Remedial Investigation/Feasibility Study efforts.

Table B-7. Estimated average Cs-137 (pC/g) for “cohesive” sediment areas of GBTOX model segments.

Cs-137 (pC/g)									
GBTOX segment									
Layer	1	2	3	4	5	6	7	8	9
0-2 cm	0.8898	0.8656	0.9872	2.4177	2.2494	4.2725	6.9114	8.9183	8.8770
2-4 cm	1.1792	1.0206	1.1841	2.3828	1.8608	3.6585	4.4715	8.4500	6.4147
4-6 cm	1.1941	0.9986	1.1581	2.0487	1.6911	4.2180	4.5574	8.3381	4.8037
6-10 cm	1.3532	0.9809	1.2716	1.7225	1.6594	3.8140	3.9469	6.9369	2.7195
> 10 cm	0.2750	0.2760	0.2959	0.3393	0.4622	0.6104	1.0992	0.8350	0.8543

Table B-8. Estimated average Pb-210 (pC/g) for “cohesive” sediment areas of GBTOX model segments.

Pb-210 (pC/g)									
GBTOX segment									
Layer	1	2	3	4	5	6	7	8	9
0-2 cm	1.8637	1.6058	1.8766	3.1819	2.7112	4.2790	16.226	13.9017	16.4451
2-4 cm	1.7607	1.4906	1.7431	3.1612	2.5500	4.5207	9.1990	12.7313	11.6791
4-6 cm	1.6873	1.3375	1.6545	2.8683	2.3477	4.0483	8.4388	11.6913	9.4358
6-10 cm	1.5265	1.1696	1.5189	1.9884	2.3204	3.9382	5.3038	9.5420	10.0971
> 10 cm	0.2930	0.3186	0.3609	0.7211	0.8775	0.9746	1.9504	2.6841	19.9474